On the Inverse Scattering Problem for the Helmholtz Equation in One Dimension

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Interest in the numerical solution of acoustic inverse scattering problems arises in a number of areas. Examples include medical diagnostics, non-destructive industrial testing, geophysical prospecting for petroleum and minerals, and detection of earthquakes.

The highly nonlinear and oscillatory nature of the problem is one of the major difficulties one encounters in the construction of effective inversion algorithms. Schemes based on global or local linearization methods, or nonlinear optimization techniques, tend to work only when the index of refraction is almost constant. They develop serious convergence problems whenever the perturbation of the index of refraction increases.

Limited successes in the solution of the inverse problems have been achieved only in one dimensional cases (Gelfand-Levitan and layer striping methods are among the most notable). These methods are generally unstable numerically since the procedures used to calculate the index of refraction are ill-conditioned.

We present a method for the solution of inverse problems for the one dimensional Helmholtz equation. The scheme is based on a combination of the standard Riccati equation for the impedance function with a new trace formula for the derivative of the index of refraction, and can be viewed as a frequency domain version of the layer-stripping approach. The principal advantage of the procedure is that if the scatterer to be reconstructed has $m \geq 1$ continuous derivatives, the accuracy of the reconstruction is proportional to $1/a^m$, where a is the highest frequency for which scattering data are available. Thus, a smooth scatterer is reconstructed very accurately from a limited amount of available data.

The scheme has an asymptotic cost $O(n^2)$, where n is the number of features to be recovered (as do classical layer-stripping algorithms), and is stable with respect to perturbations of the scattering data. The performance of the algorithm is illustrated by several numerical examples. Generalizations of this approach in two dimensions are discussed.

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Chapter 1

Introduction

1.1 Background

During the last several decades, the inverse scattering problems for the Helmholtz equation have enjoyed a remarkable degree of popularity, both in pure and applied contexts (see, e.g., [1], [2]). A number of algorithms has been proposed for the numerical treatment of these problems, in such environments as medical diagnostics, non-destructive industrial testing, anti-submarine warfare, oil exploration, etc. In the design of such a scheme, three major problems have to be overcome.

1. The problem is highly non-linear, even in its purely mathematical form. In the one-dimensional case, the problem can be reduced to a linear one, but the procedure is not stable numerically.

2. Once a mathematically valid inversion scheme is constructed, it might or might not be stable numerically. In fact, no numerically robust schemes seem to exist at this time, except in one dimension.

3. The cost of applying the scheme on the computer tends to be extremely high, except in the one-dimensional case.

The existing attempts to solve inverse scattering problems for the Helmholtz equation can be roughly subdivided into four groups.

1. Linearized inversion schemes, attempting to approximate the inverse scattering problem by the problem of inverting an appropriately chosen linear operator (see, for example, [2]).

2. Methods based on the non-linear optimization techniques, attempting to recover the parameters of the problem iteratively, by solving a sequence of forward scattering problems (see, for example, [3], [4], [5]).

3. Gel'fand-Levitan and related techniques, converting the Helmholtz equation into the Schrödinger equation, the inverse problem for the latter being reducible to the solution of a linear Volterra integral equation (see, for example, [1], [6]).

4. Techniques based on the so-called trace formulae, connecting the high frequency behavior of the solutions of the Helmholtz equation with the local values of the parameters to be recovered (see, for example, [7], [8], [9]).

The approach of this thesis falls into the category 4 above, and is different from the preceding work in the choice of the trace formula (see Theorem 4.19 in Section 4.3). The new trace formula leads to an algorithm with superior convergence properties for smooth scatterers (see Chapter 5 below), and the resulting numerical procedure is extremely stable and efficient.

1.2 Thesis Organization

Chapter 2 contains the exact formulation of the problem to be addressed, together with the relevant notation. In Chapter 3, we summarize the background facts to be used in this thesis. Chapter 4 is devoted to the development of the mathematical apparatus used to construct the algorithm, and in Chapter 5 the scheme itself is presented. In Chapter 6 we present several numerical examples demonstrating the actual performance of the procedure. Finally, in Chapter 7 we discuss generalizations of the approach to higher dimensions.

Chapter 2

Formulation of the Problem

2.1 The Helmholtz Equation

Following the standard practice, we will be considering the one dimensional scalar Helmholtz equation

$$\phi''(x,k) + k^2(1+q(x))\phi(x,k) = 0. \tag{2.1}$$

Unless specified otherwise, we will be assuming that $q \in c_0^2([0,1])$, i.e., that q is twice continuously differentiable everywhere, and that $q(x) = 0$ for all $x \notin [0,1]$. Defining the function $n : R \to R$ by the formula

$$n(x) = \sqrt{1+q(x)}, \tag{2.2}$$

we will denote by n_0, n_1 the minimum and maximum of n respectively, and assume that $0 < n_0$ so that

$$n_0 \le n(x) = \sqrt{1+q(x)} \le n_1. \tag{2.3}$$

For any complex k, we consider solutions of the Helmholtz equation $\phi_+(x,k)$ and $\phi_-(x,k)$ which have the form

$$\begin{aligned} \phi_+(x,k) &= \phi_{inc+}(x,k) + \phi_{scat+}(x,k), & (2.4) \\ \phi_-(x,k) &= \phi_{inc-}(x,k) + \phi_{scat-}(x,k) & (2.5) \end{aligned}$$

with

$$\begin{aligned} \phi_{inc+}(x,k) &= e^{ikx}, & (2.6) \\ \phi_{inc-}(x,k) &= e^{-ikx} & (2.7) \end{aligned}$$

and $\phi_{scat+}, \phi_{scat-}$ both satisfying the outgoing radiation boundary conditions

$$\phi'_{scat}(0,k) + ik\phi_{scat}(0,k) = 0, \tag{2.8}$$
$$\phi'_{scat}(1,k) - ik\phi_{scat}(1,k) = 0. \tag{2.9}$$

Normally, ϕ_{inc+} and ϕ_{inc-} are referred to as right-going and left-going incident fields respectively, and ϕ_{scat+} and ϕ_{scat-} are called scattered fields corresponding to the excitations ϕ_{inc+} and ϕ_{inc-}. The sum of an incident field and its corresponding scattered field is called the total field.

Remark 2.1 *Throughout this thesis, given a function $f(x,k)$, we will take the liberty to denote $\frac{\partial f}{\partial x}$ by $f'(x,k)$, so that the derivatives in the formulae (2.15), (2.16) are with respect to x.*

As is well-known, for any complex k, the scattered fields $\phi_{scat+}(x,k)$ and $\phi_{scat-}(x,k)$ satisfy the nonhomogeneous Helmholtz equations

$$\phi''_{scat+}(x,k) + k^2(1+q(x))\phi_{scat+}(x,k) = -k^2 q(x)e^{ikx}, \tag{2.10}$$
$$\phi''_{scat-}(x,k) + k^2(1+q(x))\phi_{scat-}(x,k) = -k^2 q(x)e^{-ikx}. \tag{2.11}$$

Since $q(x) = 0$ for all $x \notin (0,1)$, it is easy to see that for any $k \in C$ there exist two complex numbers $\mu_+(k), \mu_-(k)$, identified as the reflection coefficients, such that

$$\phi_{scat}(x,k) = \mu_+(k)\cdot e^{-ikx}, \textit{ for all } x \le 0, \tag{2.12}$$
$$\phi_{scat}(x,k) = \mu_-(k)\cdot e^{ikx}. \textit{ for all } x \ge 1, \tag{2.13}$$

due to (2.10), (2.8) and (2.11), (2.9) respectively.

2.2 The Impedance Functions

Denote by C^+ the upper half of the complex plane so that

$$C^+ = \{k \in C | Im(k) \ge 0\}. \tag{2.14}$$

For any $k \in C^+$, the impedance functions $p_+(x,k), p_-(x,k)$ associated with $\phi_+(x,k), \phi_-(x,k)$, respectively, are defined by the formulae

$$p_+(x,k) = \frac{\phi'_+(x,k)}{ik\phi_+(x,k)}, \tag{2.15}$$
$$p_-(x,k) = \frac{\phi'_-(x,k)}{-ik\phi_-(x,k)}. \tag{2.16}$$

Remark 2.2 *For x outside the scatterer. it is easy to obtain explicit expressions for p_+, p_- in terms of reflection coefficients μ_+, μ_-. Indeed, combining (2.4) with (2.12), (2.5) with (2.13), we have*

$$\phi_+(x,k) = e^{ikx} + \mu_+(k)e^{-ikx}, \text{ for all } x \leq 0, \tag{2.17}$$
$$\phi_-(x,k) = e^{-ikx} + \mu_-(k)e^{ikx}, \text{ for all } x \geq 1, \tag{2.18}$$

which can be reformulated as

$$\phi_+(x,k) = e^{ikx} + b_+(k)e^{-ikx+\alpha_+(k)}, \text{ for all } x \leq 0, \tag{2.19}$$
$$\phi_-(x,k) = e^{-ikx} + b_-(k)e^{ikx+\alpha_-(k)}, \text{ for all } x \geq 1. \tag{2.20}$$

with $\alpha_+(k), \alpha_-(k)$ real numbers and $b_+(k) \geq 0$, $b_-(k) \geq 0$, for any $k \in C$. Consequently,

$$p_+(x,k) = \frac{1 - b_+^2(k) + i2b_+(k)\sin(kx - \alpha_+(k))}{1 + b_+^2(k) + 2b_+(k)\cos(kx - \alpha_+(k))} \tag{2.21}$$

for all $x \leq 0$, and

$$p_-(x,k) = \frac{1 - b_-^2(k) + i2b_-(k)\sin(kx - \alpha_-(k))}{1 + b_-^2(k) + 2b_-(k)\cos(kx - \alpha_-(k))} \tag{2.22}$$

for all $x \geq 1$.

For any complex number k, the boundary value problems for ϕ_+, ϕ_- can be reformulated as initial value problems. More specifically, formulae (2.4), (2.5), (2.12) and (2.13) imply that there exist such complex constants α, β, depending only on k, that

$$\phi_+(x,k) = \alpha \cdot e^{ikx}, \text{ for all } x \geq 1, \tag{2.23}$$
$$\phi_-(x,k) = \beta \cdot e^{-ikx}, \text{ for all } x \leq 0. \tag{2.24}$$

Furthermore, α, β are nonzero because, e.g., if $\beta = 0$, then $\phi_-(0,k) = \phi'_-(0,k) = 0$, according to uniqueness theorem on initial value problems, $\phi_-(x,k) = 0$ for all $x \in R$, i.e.,

$$\phi_{scat-}(x,k) = -\phi_{inc-}(x,k) = -e^{-ikx}, \tag{2.25}$$

contradicting to (2.13). Clearly, formulae (2.23), (2.24) can be used as initial conditions for equation (2.1) to (uniquely) determine the total fields ϕ_+, ϕ_-.

Remark 2.3 *While the existence and uniqueness of the functions ϕ_+, ϕ_- are quite obvious for any complex k, the functions $p_+(x,k). p_-(x,k)$ are only well-defined when $Im(k) \geq 0$, and the proof of this fact is somewhat involved (see lemmas in Section 4.1 below).*

Remark 2.4 *It is easy to see that the impedance functions p_+, p_- are independent of the nonzero coefficients α, β in (2.23), (2.24). Therefore, for simplicity, the initial conditions (2.23), (2.24) are reformulated as*

$$\phi_+(x,k) = e^{ikx}, \ for\ all\ x \geq 1, \tag{2.26}$$
$$\phi_-(x,k) = e^{-ikx}. \ for\ al\ x \leq 0 \tag{2.27}$$

The functions ϕ_+, ϕ_- as solutions of equation (2.1) subject to boundary conditions (2.26), (2.27) differ from those subject to boundary conditions (2.23), (2.24) by constants.

The classical inverse scattering problem for the equation (2.1) is as follows:
Problem 1. Given the impedance function $p_+(0,k)$ for all $k \in R$, reconstruct the potential q for all $x \in [0,1]$.

It is well-known that this problem has a unique solution (and in the class of functions q much broader than $c_0^2([0,1])$, and several constructive schemes for that purpose have been proposed, most notably the Gel'fand-Levitan and related methods. However, in applications the impedance function $p_+(0,k)$ is measured with a finite accuracy and at a finite number of (usually equispaced) values of the wavenumber k. Therefore, the following problem is more relevant in numerical applications

Problem 2. Suppose that the impedance function $p_+(0,k)$ is given at a finite number of frequencies $k_j, j = 1,2,\ldots,N$ defined by the formulae $k_j = j \cdot h$, with h a positive constant. Suppose further that the values $p_+(0,k_j)$ are given with the relative accuracy ϵ. Reconstruct the potential q in the interval $[0,1]$ with the error that rapidly decreases with increasing N and decreasing h.

This thesis is devoted to the construction of an algorithm for the solution of the Problem 2.

Observation 2.5 *The value of impedance function p_+ at $x = x_0$, $x_0 \leq 0$ can be obtained from $\phi_+(x_0,k)$ in the following manner. Assuming that at $x \leq 0$, the total field $\phi_+(x,k)$ is given by (2.17), from which $\mu_+(k)$ can be obtained*

$$\mu_+(k) = \left(\phi_+(x_0,k) - e^{ikx_0}\right) e^{ikx_0}, \tag{2.28}$$

the value of the impedance function p_+ at $x = x_0$ is then

$$p_+(x_0,k) = \frac{\phi'_+(x_0,k)}{ik\phi_+(x_0,k)} = \frac{1-\mu_+(k)e^{-2ikx_0}}{1+\mu_+(k)e^{-2ikx_0}} \tag{2.29}$$
$$= 2\frac{e^{ikx_0}}{\phi_+(x_0,k)} - 1. \tag{2.30}$$

Similarly, for any $x_1 \geq 1$,

$$p_-(x_1,k) = \frac{1-\mu_-(k)e^{2ikx_1}}{1+\mu_-(k)e^{2ikx_1}} = 2\frac{e^{-ikx_1}}{\phi_-(x_1,k)} - 1. \tag{2.31}$$

Chapter 3

Mathematical Preliminaries

In this chapter, we summarize several well-known mathematical facts to be used in the rest of this thesis. These facts are given without proofs, since Lemmas 3.1–3.8 are found in standard textbooks (see, for example, [10], [11],) and Lemmas 3.9–3.6 are easy to verify directly.

3.1 Basic Lemmas

The following basic facts are tailored and stated in such a way that they will be directly used in the existence and convergence proofs, see Chapter 4 and Section 5.2.

Lemma 3.1 *Suppose that A is a linear mapping $C[0,1] \to C[0,1]$ and that $\|A\| \leq \rho$, with ρ a real number such that $\rho < 1$. Then for any $g \in L^2[0,1]$, the equation*

$$\phi = A\phi + g \tag{3.1}$$

has a unique solution, which is the sum of the series (known as Neumann's series)

$$\phi = \sum_{j=0}^{\infty} A^j g. \tag{3.2}$$

Furthermore,

$$\|\phi - \sum_{j=0}^{n} A^j g\| \leq \frac{\rho^{n+1}}{1-\rho}\|g\|. \tag{3.3}$$

Lemma 3.2 *Suppose that $f \in c_0^m([0,D])$ (i.e., f has m continuous derivatives and $f(x) = 0$ for all $x \notin (0,D)$), and that $f^{(m)}$ is absolutely continuous. Suppose further that $g \in c^{m+1}(R)$, $g^{(m+1)}$ is absolutely continuous and there exist real*

number $a > 0$ such that $g'(x) \geq a$ for all $x \in R$. Then there exists a real $c > 0$ such that

$$\left|\int_0^D f(x)e^{ik(x+g(x))}dx\right| < \frac{c}{|k|^{m+1}} \tag{3.4}$$

for all complex k such that $Im(k) \geq 0$.

Lemma 3.3 *Suppose that $f \in c^l(R)$ with l a nonnegative integer. Suppose further that $f^{(j)}(0) = 0$ for $0 \leq j \leq l$, $f^{(l)}$ is absolutely continuous Then there exists a positive number c such that*

$$\int_0^x f(t)e^{ik(x-t)}dt = -\sum_{j=1}^{l}\left(\frac{1}{2ik}\right)^j f^{j-1}(x) + \left(\frac{1}{2ik}\right)^{l+1}(f^l(x) + b(x,k)) \tag{3.5}$$

with $b : R \times C^+ \to C$ an absolutely continuous function of $x \in [0,1]$ such that

$$|b(x,k)| \leq c. \tag{3.6}$$

for all $x \in [0,1]$, $k \in C^+$. Furthermore, if $f(x) = 0$ for all $x \geq D$ with D a positive number, then

$$|b(x,k)| \leq c. \tag{3.7}$$

for all $(x,k) \in R \times C^+$

Lemma 3.4 *Suppose that $a : [0,1] \to R$ and $b : [0,1] \to C$ are two continuous functions, and that $a(x) > 0$, for all $x \in [0,1]$. Then for any two solutions u and v of the second order ODE*

$$(a(x)\phi'(x))' + b(x)\phi(x) = 0, \tag{3.8}$$

there exists a constant c such that

$$a(x)(u(x)v'(x) - v(x)u'(x)) = c \tag{3.9}$$

for all $x \in [0,1]$. Furthermore, $c \neq 0$ if and only if u and v are linearly independent. (The expression $W(u,v) = u(x)v'(x) - v(x)u'(x)$ is referred to as the Wronskian of the pair u, v).

Lemma 3.5 *(Gronwall's inequality) Suppose that $u, v, w : [0,a] \to R$ are three continuous and nonnegative functions, satisfying the inequality*

$$w(x) \leq u(x) + \int_0^x v(t)w(t)dt \tag{3.10}$$

for all $x \in [0,a]$. Then

$$w(x) \leq u(x) + \int_0^x u(t)v(t)e^{\int_t^x v(\tau)d\tau}dt \tag{3.11}$$

for all $x \in [0,a]$.

The following lemma is a special case of the general theorem about continuous dependence on initial conditions and parameters of solutions of ODEs (see, for example, [11]).

Lemma 3.6 *Suppose that $a : C \to C$ is an entire function and that $A : R \times C \to C^{n\times n}$ is an $n \times n$-matrix whose entries $a_{i,j}(x,z), i,j = 1,\ldots,n$ are continuous functions of x and entire functions of z for all $x \in R$. Then for any $z \in C$, the differential equation*

$$y'(x,z) = A(x,z)\cdot y(x,z) \tag{3.12}$$

subject to the initial condition

$$y(0) = c(z) \tag{3.13}$$

has an unique solution $y(x,z)$ for all $x \in R$. Moreover, $y(x,z)$ is an entire function of z.

3.2 Schrödinger Equation and Riccati Equation

Lemmas 3.7– 3.13 describe the basic facts about the Helmholtz equation and its connections with the Schrödinger Equation and the Riccati Equation, in the context of scattering problems.

Lemma 3.7 *Suppose that $G_k : [0,1] \times [0,1] \to C$ is the Green's function of the boundary value problem*

$$\psi''(x,k) + k^2\psi(x,k) = 0, \tag{3.14}$$

$$\psi'(0,k) + ik\psi(0,k) = 0, \tag{3.15}$$

$$\psi'(1,k) - ik\psi(1,k) = 0. \tag{3.16}$$

for any complex $k \neq 0$. Then the boundary value problem

$$\psi''(x,k) + (k^2 + \eta(x))\psi(x,k) = f(x,k) \tag{3.17}$$

$$\psi'(0,k) + ik\psi(0,k) = 0, \tag{3.18}$$

$$\psi'(1,k) - ik\psi(1,k) = 0. \tag{3.19}$$

is equivalent to a second kind integral equation

$$\psi(x,k) = -\int_0^1 G_k(x,t)\eta(t)\psi(t,k)dt + g(x,k) \tag{3.20}$$

with $f, g : [0,1] \times C \to C$ and g defined by the formula

$$g(x,k) = \int_0^1 G_k(x,t)f(t,k)dt. \tag{3.21}$$

Lemma 3.8 *For any complex $k \neq 0$, the Helmholtz equation*

$$\psi''(x,k) + k^2\psi(x,k) = 0 \tag{3.22}$$

with the outgoing radiation conditions (2.8) (2.9) has the Green's function

$$G_k(x,t) = \frac{1}{2ik}\begin{cases} e^{ik(t-x)}, & x \leq t, \\ e^{ik(x-t)}, & x \geq t. \end{cases} \tag{3.23}$$

Lemma 3.9 *Suppose that $q : R \to R$ is a c^2–function such that $q > -1$ for all $x \in R$. Suppose further that the functions $n, x, S, \eta, g : R \to R$ are defined by the formulae*

$$n(x) = \sqrt{1 + q(x)}, \tag{3.24}$$

$$t(x) = \int_0^x n(\tau)d\tau, \tag{3.25}$$

$$S(t) = (1 + q(x(t)))^{\frac{-1}{4}} \tag{3.26}$$

$$\begin{aligned} \eta(t) &= \frac{S''(t)}{S(t)} - \frac{n'(x)}{2(n(x))^2} \\ &= \frac{1}{4}(1+q)^{-2}\left(q''(x) - \sqrt{1+q(x)}q'(x) - \frac{5}{4}(1+q)^{-1}q'^2(x)\right) \end{aligned} \tag{3.27}$$

$$g(t) = \frac{f(x)}{S(t)} = f(x) \cdot (1 + q(x))^{\frac{1}{4}} \tag{3.28}$$

Finally, suppose that the function $\phi : R \times C \to C$ satisfies the equation

$$\phi''(x,k) + k^2(1 + q(x)) \cdot \phi(x,k) = f(x), \tag{3.29}$$

and the function $\psi : R \times C \to C$ is defined by the formula

$$\psi(t,k) = \phi(x(t),k)/S(t) = \phi(x,k) \cdot (1 + q(x))^{\frac{1}{4}} \tag{3.30}$$

Then the function ψ satisfies the Schrödinger equation

$$\psi''(t,k) + (k^2 + \eta(t)) \cdot \psi(t,k) = g(t). \tag{3.31}$$

at all $t \in R$.

Remark 3.10 *Lemma 3.9 provides a connection between the solutions of the Helmholtz equation (3.29) and those of the appropriately chosen Schrödinger equation (3.31). This connection will be used in the following chapter as an analytical tool. However, it is not useful in numerical computations since the connection between η and q (see (3.27)) is generally ill-conditioned.*

Corollary 3.11 *Suppose that under the conditions of the preceding lemma that* $q(x) = 0$ *for all* $x \notin (0,1)$. *Suppose further that the functions* $\psi_+, \psi_- : R \times C \to C$ *are defined by the formulae*

$$\psi_+(t,k) = \phi_+(x(t),k)/S(t), \tag{3.32}$$
$$\psi_-(t,k) = \phi_-(x(t),k)/S(t). \tag{3.33}$$

Then ψ_+, ψ_- *satisfy the ODEs*

$$\psi_+''(t,k) + (k^2 + \eta(t)) \cdot \psi_+(t,k) = 0, \tag{3.34}$$
$$\psi_-''(t,k) + (k^2 + \eta(t)) \cdot \psi_-(t,k) = 0 \tag{3.35}$$

subject to the boundary conditions

$$\psi_+(t,k) = \xi(k) \cdot e^{ik(t-T_1)} \tag{3.36}$$

for all $t \geq T_1$, *and*

$$\psi_-(t,k) = e^{-ikt} \tag{3.37}$$

for all $t \leq 0$ *with* $T_1 > 0$, $\xi(k) \neq 0$ *defined by the formulae*

$$T_1 = t(1) = \int_0^1 n(\tau)d\tau, \tag{3.38}$$
$$\xi(k) = S(T_1)e^{ik}. \tag{3.39}$$

Furthermore,

$$p_+(x,k) = n(x)\frac{\psi_+'(t,k)}{ik\psi_+(t,k)} - \frac{n'(x)}{2ikn(x)}, \tag{3.40}$$
$$p_-(x,k) = n(x)\frac{\psi_-'(t,k)}{-ik\psi_-(t,k)} + \frac{n'(x)}{2ikn(x)}. \tag{3.41}$$

Observation 3.12 *Suppose that* $q(x) = 0$ *for all* $x \notin (0,1)$. *Then according to Lemma 3.9 and Corollary 3.11,*

$$t = x, \tag{3.42}$$
$$S(t) = 1, \tag{3.43}$$

and consequently

$$\phi_+(x,k) = \psi_+(t,k) \tag{3.44}$$

for all $x \leq 0$. *Now, suppose the function* ψ_+ *is defined by formulae (3.32), (2.17). Defining the scattered field* $\psi_{scat+} : R \times C \to C$ *by the formula*

$$\psi_+(t,k) = e^{ikt} + \psi_{scat+}(t,k), \tag{3.45}$$

we immediately see that

$$\psi_{scat+}(t,k) = \mu_+(k) \cdot e^{-ikt} \tag{3.46}$$

for all $x \leq 0$ *due to (3.44), (2.17), (3.45). Finally, combining (3.45) with (3.34), we observe that* ψ_{scat+} *satisfies the Schrödinger equation*

$$\psi''_{scat+}(t,k) + (k^2 + \eta(t))\psi_{scat+}(t,k) = \frac{-k^2 q(x(t)) e^{ikx(t)}}{S(t)} \tag{3.47}$$

subject to outgoing radiation conditions (2.8), (2.9) (the latter due to (3.46), (3.36)).

Lemma 3.13 *Suppose that under the conditions of the preceding lemma,*

$$\begin{aligned} \phi_+(x_0,k_0) &\neq 0, && (3.48)\\ \phi_-(x_0,k_0) &\neq 0 && (3.49) \end{aligned}$$

at some point $(x_0,k_0) \in R \times C$*. Then there exists a neighborhood* D *of* (x_0,k_0) *such that the impedance functions* p_+, p_- *satisfy the Riccati equations*

$$\begin{aligned} p'_+(x,k) &= -ik(p_+^2(x,k) - (1+q(x)), && (3.50)\\ p'_-(x,k) &= ik(p_-^2(x,k) - (1+q(x)) && (3.51) \end{aligned}$$

for all $(x,k) \in D$.

Observation 3.14 *Combining formulae (2.23), (2.24), we easily observe that*

$$\begin{aligned} p_+(x,k) &= 1, \text{ for all } x \geq 1, && (3.52)\\ p_-(x,k) &= 1, \text{ for all } x \leq 0, && (3.53) \end{aligned}$$

for all complex $k \neq 0$.

Chapter 4

Impedance Functions and Their Properties

In this chapter, we investigate analytical properties of the impedance functions p_+, p_-. Our principal purpose here is to formulate exactly and prove the following three facts.

(1) For any $x \in R$, the impedance functions $p_+(x,k), p_-(x,k)$ are analytic functions of k in the upper half plane C^+. Furthermore,

$$p_+(x,k) = \sqrt{1+q(x)} - \frac{q'(x)}{4(1+q(x))} \cdot \frac{1}{ik} + O(k^{-2}), \tag{4.1}$$

$$p_-(x,k) = \sqrt{1+q(x)} + \frac{q'(x)}{4(1+q(x))} \cdot \frac{1}{ik} + O(k^{-2}), \tag{4.2}$$

for all $x \in R$, $k \in C^+$ (see Theorem 4.14 below).

(2) For large real k, the difference between $\overline{p_+}$ and p_- is extremely small (it decays like k^{-m}, where m is the smoothness of the scatterer, see Theorem 4.18 below). The expressions (4.1), (4.2) are the first two terms in WKB expansions of the functions p_+, p_-, respectively.

(3) For any $a > 0$, and all $x \in R$, we have the so-called trace formula

$$q'(x) = \frac{2}{\pi}(1+q(x)) \int_{-a}^{a} (p_+(x,k) - p_-(x,k))dk + O(a^{-(m-1)}), \tag{4.3}$$

with m the smoothness of the scatterer (see Theorem 4.19 below).

As often happens, the statements (1)–(3) above have extremely simple formulations, and a transparent physical interpretation. However, their proofs are technical and do not follow any simple physical intuition.

4.1 Boundedness

The following five lemmas establish the basic properties of the impedance functions p_+, p_- introduced in Chapter 1. Lemma 4.1 is a technical one, describing the behavior of ϕ_+, ϕ_- in the vicinity of $k = 0$ in the complex plane. Lemma 4.2 describes the properties of the impedance functions p_+, p_- near $k = 0$, Lemma 4.4 demonstrates the well-definedness of the impedance functions for real k, and Lemmas 4.5 and 4.6 provide upper and lower bounds for the impedance functions.

Lemma 4.1 *Suppose that $q \in c([0,1])$ and $A > 0$ is a real number. Then there exist three positive numbers δ, α and β such that*

$$1. \quad |\phi_+(x,k) - 1| \leq \alpha |k|, \tag{4.4}$$
$$2. \quad |\phi_-(x,k) - 1| \leq \alpha |k|, \tag{4.5}$$
$$3. \quad |\phi'_+(x,k) - ik| \leq \beta |k|^2, \tag{4.6}$$
$$4. \quad |\phi'_-(x,k) + ik| \leq \beta |k|^2, \tag{4.7}$$
$$5. \quad \phi_+(x,k) \neq 0, \tag{4.8}$$
$$6. \quad \phi_-(x,k) \neq 0, \tag{4.9}$$

for all real $x \in [-A, A]$ and complex k such that $|k| < \delta$.

Proof. Since the proofs of this lemma for ϕ_+, ϕ'_+ and for ϕ_-, ϕ'_- are identical, we only prove it in the case of ϕ_-, ϕ'_-. Defining two auxiliary functions $\phi_1, \psi : R \times C \to C$ by the formulae

$$\begin{aligned} \phi_1(x,k) &= \phi_-(x,k) - 1, && (4.10) \\ \psi(x,k) &= \phi'_-(x,k) + ik, && (4.11) \end{aligned}$$

and combining (4.10), (4.11) with equation (2.1) and the initial condition (2.27), we observe that the functions ϕ_1, ψ satisfy the linear first order ODEs

$$\begin{aligned} \phi'_1(x,k) &= \psi(x,k) + ik, && (4.12) \\ \psi'(x,k) &= -k^2(1+q(x))(1+\phi_1(x,k)) && (4.13) \end{aligned}$$

subject to the initial conditions

$$\begin{aligned} \phi_1(0,k) &= 0, && (4.14) \\ \psi(0,k) &= 0. && (4.15) \end{aligned}$$

We start with showing that there exist continuous functions $M,\ N : R^+ \times R^+ \to R^+$ such that, for any $s \in R^+$, $M(s,t)$, $N(s,t)$ are monotonically increasing functions of t for all $t \in R^+$ and

$$\begin{aligned} |\phi_1(x,k)| &\leq M(A,|k|)|k|, && (4.16) \\ |\psi(x,k)| &\leq N(A,|k|)|k|^2. && (4.17) \end{aligned}$$

First, we prove the estimate (4.17). Integrating (4.12) from 0 to x, we have

$$\phi_1(x,k) = \int_0^x (ik + \psi(t,k))dt, \tag{4.18}$$

and substituting (4.18) into (4.13) and integrating the result of the substitution, obtain

$$\psi(x,k) = -k^2 \int_0^x (1+q(t)) \left(1 + \int_0^t (ik + \psi(\tau,k))d\tau\right) dt. \tag{4.19}$$

Denoting $|\psi(x,k)|$ by $a(x,k)$ and observing that $1 + q(x) \leq n_1^2$ (see (2.3) in Section 2.1), we obtain

$$\begin{aligned} a(x,k) &\leq |k|^2 n_1^2 \left(|x| + \frac{1}{2}x^2|k| + \int_0^x \int_0^t a(\tau,k)d\tau dt\right) \\ &\leq |k|^2 n_1^2 \left(|x| + \frac{1}{2}x^2|k|\right) + |k|^2 n_1^2 \int_0^x (x-t)a(t,k)dt \end{aligned} \tag{4.20}$$

for any $x \in R$. Gronwall's inequality (see Lemma 3.5) implies that for any $x \in [0, A]$,

$$\begin{aligned} a(x,k) &\leq |k|^2 n_1^2 \left(|x| + \frac{1}{2}x^2|k| + \int_0^x |t| + \frac{1}{2}t^2|k|(x-t)e^{\frac{1}{2}(x-t)^2}dt\right) \\ &\leq N(A,|k|)|k|^2. \end{aligned} \tag{4.21}$$

It is easy to see that (4.21) is also valid for any $x \in [-A, 0]$, and we obtain the estimate (4.17) with $N(A,k)$ defined by the formula

$$N(A,|k|) = \sup_{-A<x<A} n_1^2 \left(|x| + \frac{1}{2}x^2|k| + \int_0^x |t| + \frac{1}{2}t^2|k|(x-t)e^{\frac{1}{2}(x-t)^2}dt\right). \tag{4.22}$$

We now turn our attention to the estimate (4.16). Substituting (4.17) into (4.18), we obtain

$$\begin{aligned} |\phi_1(x,k)| &\leq |x|\left(|k| + N(A,|k|)|k|^2\right) \\ &\leq M(A,|k|)|k|, \end{aligned} \tag{4.23}$$

with

$$M(A,|k|) = A(1 + |k|N(A,|k|)), \tag{4.24}$$

for all real $x \in [-A, A]$ and complex k, which proves (4.16).

Now, the estimates (4.5) and (4.7) easily follow from (4.16) and (4.17). Indeed, since $M(A,t)$ is a continuous, monotonically increasing function of t, there exists a real δ such that

$$M(A,\delta) \cdot \delta < 1. \tag{4.25}$$

Denoting $M(A,\delta)$ by α, $N(A,\delta)$ by β and observing that $M(A,|k|), N(A,|k|)$ are monotonically increasing functions of $|k|$, we have

$$
\begin{aligned}
|\phi_1(x,k)| &\le M(A,|k|)|k| \le M(A,\delta)|k| = \alpha|k|, && (4.26)\\
|\psi(x,k)| &\le N(A,|k|)|k| \le N(A,\delta)|k| = \beta|k|^2, && (4.27)
\end{aligned}
$$

from which (4.5), (4.7) follow immediately.

Finally, (4.9) is a direct consequence of (4.26) and (4.25). □

Lemma 4.2 *Suppose that $q \in c_0^2([0,1])$ and $A > 0$ is a real number. Then there exists $\delta > 0$ such that the impedance functions p_+, p_- are continuous functions of (x,k) for all real $(x,k) \in D$ with*

$$D = \{(x,k) | x \in [-A,A], k \in C, k \neq 0, |k| \le \delta\} \tag{4.28}$$

Furthermore,

$$
\begin{aligned}
\lim_{k\to 0} p_+(x,k) &= 1, && (4.29)\\
\lim_{k\to 0} p_-(x,k) &= 1. && (4.30)
\end{aligned}
$$

Proof. Due to Lemma 4.1, there exists a positive number δ such that $\phi_+(x,k) \neq 0$, $\phi_-(x,k) \neq 0$ for all real $(x,k) \in D$. Therefore, the functions p_+, p_- are well-defined in D, and their continuity follows from the continuity of ϕ_+, ϕ'_+, ϕ_-, ϕ'_- and the formulae (2.15), (2.16). Finally, (4.29), (4.30) are direct consequences of Formulae (4.4)– (4.7). □

Remark 4.3 *While the impedance functions p_+, p_- are continuous in the vicinity of $k = 0$ in the complex plane, formulae (2.15), (2.16) fail to define p_+, p_- at $k = 0$. We now can define $p_+(x,0) = p_-(x,0) = 1$ for all $x \in R$ due to Lemma 4.2.*

Lemma 4.4 *For any real $k \neq 0$ and all $x \in R$*

$$
\begin{aligned}
\phi_+(x,k) &\neq 0, && (4.31)\\
\phi'_+(x,k) &\neq 0, && (4.32)\\
\phi_-(x,k) &\neq 0, && (4.33)\\
\phi'_-(x,k) &\neq 0. && (4.34)
\end{aligned}
$$

Proof. Again, since the proofs of this lemma for ϕ_+, ϕ'_+ and for ϕ_-, ϕ'_- are identical, we only prove (4.33) and (4.34). Denoting the real part of ϕ_- by u and the imaginary part by v, so that

$$
\begin{aligned}
\phi_-(x,k) &= u(x,k) + iv(x,k), && (4.35)\\
\phi'_-(x,k) &= u'(x,k) + iv'(x,k), && (4.36)
\end{aligned}
$$

we observe that each of the functions u, v satisfies equation (2.1) (since the coefficients of the equation are real). Combining the initial condition (2.27) with (4.35), we immediately see that

$$\begin{aligned} u(x,k) &= \cos(kx), && (4.37)\\ v(x,k) &= \sin(kx) && (4.38) \end{aligned}$$

for all $x \leq 0$ and $k \neq 0$. Therefore, the Wronskian of the pair u, v is

$$W(u,v) = k, \tag{4.39}$$

for any $x \in R$ (see Lemma 3.4), and $u(x,k)$, $v(x,k)$ can not be both zero, nor can $u'(x,k)$, $v'(x,k)$, for any $x \in R$ and $k \neq 0$. Now, formulae (4.33) and (4.34) immediately follow from (4.35) and (4.36) □

We have shown that the impedance functions p_+, p_- are well-defined for all real k (see Lemmas 4.2, 4.4 and Remark (4.3)). Now, we turn our attention to the well-definedness of the impedance functions on the upper half of the k-plane. First we provide the lower bounds for p_+, p_-.

Lemma 4.5 *For all $x \in R$ and any k such that $Im(k) > 0$,*

$$\begin{aligned} Re(p_+(x,k)) &\geq n_0 \sin(\arg(k)), && (4.40)\\ Re(p_-(x,k)) &\geq n_0 \sin(\arg(k)) && (4.41) \end{aligned}$$

with $0 < n_0 \leq 1$ the minimum of $n(x)$ (see (2.3) in Section 2.1), and $\arg(k)$ the argument of the complex wave number k.

Proof. Since the proof of (4.40) and that of (4.41) are identical, we only provide the latter. Observing that

$$Re(p_-(x,k)) = p_-(x,k) = 1 > n_0^2 \sin(\arg(k)), \tag{4.42}$$

for any $Im(k) > 0$ and all $x \leq 0$ (see (3.53) in Chapter 3), we will prove (4.41) by showing that

$$\frac{\partial}{\partial x}\left(Re(p_-(x,k))\right) \geq 0 \tag{4.43}$$

for any $x > 0$ such that

$$0 \leq Re(p_-(x,k)) \leq n_0 \sin(\arg(k)) \tag{4.44}$$

(obviously, $0 < arg(k) < \pi$ for any k such that $Im(k) > 0$).

We will denote by a, b, u, v the real and imaginary parts of k and p_- respectively, so that

$$\begin{aligned} k &= a + ib, && (4.45)\\ p_-(x,k) &= u(x,k) + iv(x,k), && (4.46) \end{aligned}$$

with $b > 0$. Now, we can rewrite the Riccati equation (3.51) for p_- in the form

$$u' = b(v^2 - u^2 + n^2) - 2auv, \tag{4.47}$$

$$v' = -a(v^2 - u^2 + n^2) - 2buv. \tag{4.48}$$

We observe that $\frac{\partial}{\partial x}u(x,k)$ is a function of u, v given by the formula

$$\frac{\partial}{\partial x}u(x,k) = f(u,v) = b(v^2 - u^2 + n^2) - 2auv. \tag{4.49}$$

Denoting the interval $[0, n_0 \sin(\arg(k))]$ by I, and defining the region $D \subset R \times R$ via the formula

$$D = \{(u,v) | u \in I, v \in R\}, \tag{4.50}$$

we observe that

$$\min_{(u,v)\in D} f(u,v) = b(n^2 - n_0^2) \geq 0 \tag{4.51}$$

which proves (4.43) given (4.44). Now, (4.41) follows immediately form (4.42), (4.43) and (4.44). □

As a direct consequence of Lemma 4.5, the following lemma establishes the upper bounds of the impedance functions in the upper half-plane.

Lemma 4.6 *For any k such that $Im(k) > 0$ and all $x \in R$,*

$$|(p_+(x,k))| \leq \frac{n_1}{\sin(\arg(k))}, \tag{4.52}$$

$$|(p_-(x,k))| \leq \frac{n_1}{\sin(\arg(k))}, \tag{4.53}$$

with $n_1 > 0$ the maximum of $n(x)$ (see (2.3) in Section 2.1).

Proof. Again, we only give the proof of (4.53) since the proof for (4.52) is identical. According to Lemma 4.5, the function

$$r(x,k) = 1/p_-(x,k) \tag{4.54}$$

is well-defined for any $Im(k) > 0$. Combining (4.54) with the equation (3.51) and the boundary condition (3.53) for p_-, we observe that $r(x,k)$ obeys the Riccati equation

$$r'(x,k) = ikn^2(x)\left(r^2(x,k) - \frac{1}{n^2(x)}\right), \tag{4.55}$$

subject to the initial condition $r(0,k) = 1$. Reproducing the proof of Lemma 4.5 almost verbatim, we obtain a lower bound for the real part of r

$$Re(r(x,k)) \geq \frac{\sin(\arg(k))}{n_1}. \tag{4.56}$$

Now, the upper bound

$$|(p_-(x,k))| \le Re(r(x,k))^{-1} \le \frac{n_1}{\sin(\arg(k))} \tag{4.57}$$

is readily obtained by combining (4.54) with (4.56). □

Corollary 4.7 *For all $x \in R$ and k such that $Im(k) > 0$,*

$$\begin{aligned} \phi_+(x,k) &\ne 0, && (4.58)\\ \phi'_+(x,k) &\ne 0, && (4.59)\\ \phi_-(x,k) &\ne 0, && (4.60)\\ \phi'_-(x,k) &\ne 0. && (4.61) \end{aligned}$$

Proof. We prove this corollary by contradiction. First, we observe that

$$\phi_+(x,k) = 0 \tag{4.62}$$

implies

$$\phi'_+(x,k) = 0 \tag{4.63}$$

and vice versa, since both $\phi_+(x,k)$ and $\phi'_+(x,k)$ are continuous functions of x, and their ratio

$$ik \cdot p_+(x,k) = \frac{\phi'_+(x,k)}{\phi_+(x,k)} \tag{4.64}$$

is bounded from both above and below due to Lemmas 4.5, 4.6.

Suppose now that for some $x_0 \in R$, $Im(k_0) > 0$,

$$\phi_+(x_0,k_0) = \phi'_+(x_0,k_0) = 0. \tag{4.65}$$

Then the pair of functions

$$\begin{aligned} \phi(x) &= \phi_+(x,k_0), && (4.66)\\ \psi(x) &= \phi'_+(x,k_0) && (4.67) \end{aligned}$$

satisfies the system of ODEs

$$\begin{aligned} \phi'(x) &= \psi(x), && (4.68)\\ \psi'(x) &= -k_0^2(1+q(x))\phi(x), && (4.69) \end{aligned}$$

subject to the initial conditions

$$\phi(x_0) = \psi(x_0) = 0. \tag{4.70}$$

However, the initial value problem (4.68), (4.69), (4.70) has a unique solution

$$\phi(x) = \psi(x) = 0 \tag{4.71}$$

for all $x \le x_0$, which contradicts the condition (2.26), proving (4.58), (4.59).

The proof of (4.60), (4.61) is identical. □

Observation 4.8 *Due to Lemma 3.13, it is easy to see that*

$$\begin{aligned} \overline{p_+(x,k)} &= p_+(x,-\overline{k}), & (4.72)\\ \overline{p_-(x,k)} &= p_-(x,-\overline{k}), & (4.73) \end{aligned}$$

for all $x \in R$ and $k \in C^+$. For real k, equalities (4.72), (4.73) assume the form

$$\begin{aligned} \overline{p_+(x,k)} &= p_+(x,-k), & (4.74)\\ \overline{p_-(x,k)} &= p_-(x,-k). & (4.75) \end{aligned}$$

Indeed, combining the complex conjugate of (3.50) with that of (3.52), we obtain the ODE

$$\left(\overline{p_+(x,k)}\right)' = -i(-\overline{k})(\overline{p_+(x,k)}^2 - (1+q(x)) \tag{4.76}$$

subject to initial condition

$$\overline{p_+(0,k)} = 1. \tag{4.77}$$

Now, replacing k by $-\overline{k}$ in (3.50) and (3.52), we have

$$p_+'(x,-\overline{k}) = -i(-\overline{k})(p_+(x,-\overline{k})^2 - (1+q(x)), \tag{4.78}$$

and

$$p_+\left(0,-\overline{k}\right) = 1. \tag{4.79}$$

We notice that $\overline{p_+(x,k)}$, $p_+(x,-\overline{k})$ satisfy identical differential equations (4.76), (4.78) with identical boundary conditions (4.77), (4.79), from which (4.72) follows. A similar calculation proves (4.73).

4.2 Smoothness and Asymptotics

The following two technical lemmas describe the asymptotic behavior of the functions ψ_+, ψ_- (see Corollary 3.11 in Chapter 3), ϕ_+ and ϕ_- at large frequencies. They will be used in proofs of Theorems 4.14, 4.18, describing the high-frequency asymptotics of the impedance functions p_+, p_-. Theorems 4.14, 4.18 are in turn used in the following chapter to derive the trace formulae (4.194), (4.198), which are the principal analytical tool of this thesis.

Lemma 4.9 *Suppose that for any $a \geq 0$, the region $K(a) \subset C$ is defined by the formulae*

$$K(a) = \{k | k \in C, Im(k) \geq 0, |k| \geq a\}. \tag{4.80}$$

Suppose further that $q \in c_0^2([0,1])$, $q(x) > -1$ for all $x \in R$, and the second derivative of q is absolutely continuous. Then there exist real numbers $A >$

0, $c > 0$ such that

$$\psi_+(t,k) = \xi(k)e^{ik(t-T_1)}\left(1 + \frac{1}{2ik}\int_t^1 \eta(\tau)d\tau + \epsilon_+(t,k)\right), \tag{4.81}$$

$$\psi_+'(t,k) = ik\xi(k)e^{ik(t-T_1)}\left(1 + \frac{1}{2ik}\int_t^1 \eta(\tau)d\tau + \delta_+(t,k)\right), \tag{4.82}$$

$$\psi_-(t,k) = e^{-ikt}\left(1 + \frac{1}{2ik}\int_0^t \eta(\tau)d\tau + \epsilon_-(t,k)\right), \tag{4.83}$$

$$\psi_-'(t,k) = -ike^{-ikt}\left(1 + \frac{1}{2ik}\int_0^t \eta(\tau)d\tau + \delta_-(t,k)\right), \tag{4.84}$$

with $\xi(k) : C \to C$, $T_1 > 0$ defined by (3.39), (3.38) (see Corollary 3.11 in Chapter 3), and $\epsilon_+, \epsilon_-, \delta_+, \delta_- : R \times K(A) \to C$ continuous functions such that

$$|\epsilon_+(t,k)| \le c \cdot k^{-2}, \tag{4.85}$$

$$|\delta_+(t,k)| \le c \cdot k^{-2}, \tag{4.86}$$

$$|\epsilon_-(t,k)| \le c \cdot k^{-2}, \tag{4.87}$$

$$|\delta_-(t,k)| \le c \cdot k^{-2}. \tag{4.88}$$

for all $(t,k) \in R \times K(A)$.

Proof. Since the proofs of this lemma for ψ_+, ψ_+' and for ψ_-, ψ_-' are identical, we only prove it in the case of ψ_-, ψ_-'. Introducing two auxiliary functions $m, n : R \times C \to C$ by the formulae

$$m(t,k) = e^{ikt}\psi_-(t,k), \tag{4.89}$$

$$n(t,k) = -\frac{1}{ik}e^{ikt}\psi_-'(t,k) \tag{4.90}$$

and combining (3.35), (3.37) with (4.89), (4.90), we observe that m satisfies the equation

$$m''(t,k) - 2ikm'(t,k) = -\eta(t)m(t,k) \tag{4.91}$$

($\eta \in c_0([0,T_1])$ is absolutely continuous, see (3.27) for the definition of η) subject to the initial conditions

$$m(0,k) = 1, \tag{4.92}$$

$$m'(0,k) = 0. \tag{4.93}$$

Multiplying (4.91) by e^{-2ikt} and integrating the result from 0 to t, we have

$$m'(t,k) = -\int_0^t \eta(\tau)e^{2ik(t-\tau)}m(\tau,k)d\tau. \tag{4.94}$$

Integrating (4.94) from 0 to t, we obtain the second kind Volterra integral equation for m

$$m = F_k(m) + 1 \tag{4.95}$$

with the mapping $F_k : c(R) \to c(R)$ defined by

$$F_k(f)(t) = \frac{1}{2ik}\int_0^t \eta(\tau)(1 - e^{2ik(t-\tau)})f(\tau)d\tau. \tag{4.96}$$

Combining (4.94) with (4.89), (4.90), we observe that

$$n(t,k) = m(t,k) - \frac{1}{2ik}\int_0^t \eta(\tau)e^{2ik(t-\tau)}m(\tau,k)d\tau. \tag{4.97}$$

Since $\eta \in c_0([0,T_1])$, the function $\eta(\tau)(1 - e^{2ik(t-\tau)})$ is bounded for all real t,τ and $k \in K(0)$. Therefore, there exists a real number $c_1 > 0$ such that

$$\|F_k\| \le \frac{c_1}{|k|}, \tag{4.98}$$

and hence there exists a real number $A > 0$ such that

$$\|F_k\| \le 1 \tag{4.99}$$

for all $k \in K(A)$. Now, according to Lemma 3.1, for all $(t,k) \in R \times K(A)$, the unique solution of (4.95) can be approximated by the Neumann's series truncated at the second term

$$\begin{aligned} m(t,k) &= 1 + \frac{1}{2ik}\int_0^t \eta(\tau)(1 - e^{2ik(t-\tau)})d\tau + \alpha(t,k) \\ &= 1 + \frac{1}{2ik}\int_0^t \eta(\tau)d\tau + \beta(t,k) + \alpha(t,k) \end{aligned} \tag{4.100}$$

with $\alpha,\ \beta : R \times K(A) \to C$ such that

$$\|\alpha\| \le \frac{2c_1^2}{|k|^2} \tag{4.101}$$

(see Lemma 3.1), and

$$\beta(t,k) = -\frac{1}{2ik}\int_0^t \eta(\tau)e^{2ik(t-\tau)}d\tau. \tag{4.102}$$

Since q'' is absolutely continuous and $q(x) = 0$ for all $x \le 0$, we observe that η is absolutely continuous and $\eta(x) = 0$ for all $x \le 0$ (see (3.27) in Lemma 3.9). According to Lemma 3.3, there exists $c_2 > 0$ such that

$$|\beta(t,k)| \le \frac{c_2^2}{|k|^2}. \tag{4.103}$$

for all $x \in [0,1]$, $k \in C^+$. Now, combining (4.100) with (4.101) and (4.103), we observe that there exists $c_3 > 0$ such that

$$\left| m(t,k) - \left(1 + \frac{1}{2ik}\int_0^t \eta(\tau)d\tau\right)\right| \le \frac{c_3}{|k|^2}. \tag{4.104}$$

for all $(t,k) \in R \times K(A)$. Similarly, there exists $c_4 > 0$ such that

$$\left| n(t,k) - \left(1 + \frac{1}{2ik}\int_0^t \eta(\tau)d\tau\right)\right| \le \frac{c_4}{|k|^2} \tag{4.105}$$

due to (4.97), (4.104).

Now, (4.83), (4.87) follow immediately from (4.104), (4.92), and (4.84), (4.88) are a direct consequence of (4.105), (4.93). □

Lemma 4.10 *Suppose that $q \in c_0^\gamma([0,1])$, $\gamma \ge 2$, $q^{(\gamma)}$ is absolutely continuous and $q(x) > -1$ for all $x \in R$. Then for any integer $1 \le l \le \gamma$, the l-th interate $m_l : R \times C^+ \to C$ defined by the formulae*

$$\begin{aligned} m_0(t,k) &= 0, && (4.106)\\ m_l(t,k) &= 1 + F_k(m_{l-1})(t,k) && (4.107)\\ &= 1 + \frac{1}{2ik}\int_0^t \eta(\tau)(1 - e^{2ik(t-\tau)})m_{l-1}(\tau,k)d\tau && (4.108)\end{aligned}$$

(see (4.95), (4.96)) assumes the form

$$m_l(t,k) = 1 + \sum_{j=1}^{\gamma-1}\left(\frac{1}{2ik}\right)^j a_j(t) + \left(\frac{1}{2ik}\right)^\gamma a_\gamma(t,k) \tag{4.109}$$

with $a_j : R \to R$, $j = 1,\dots,\gamma-1$, $a_\gamma : R \times C^+ \to C$ such that

$$\frac{d^{\gamma-j}a_j(t)}{dx^{\gamma-j}} \tag{4.110}$$

are bounded and absolutely continuous for all $x \in R$, $j = 1,\dots,\gamma-1$, and

$$a_\gamma(t,k) \tag{4.111}$$

is bounded and absolutely continuous function of t for all $(t,k) \in R \times C^+$.

Proof. We prove this lemma by induction. For $l = 1$, formulae (4.106), (4.108) yield

$$m_1(t,k) = 1 \tag{4.112}$$

for all $(t,k) \in R \times C^+$, which is already in the form (4.109) satisfying conditions (4.110), (4.111).

For $l \geq 1$, assuming that $m_l(t,k)$ is in the form (4.109) satisfying conditions (4.110), (4.111), we obtain m_{l+1} using (4.108):

$$\begin{aligned} m_{l+1}(t,k) &= 1+\frac{1}{2ik}\int_0^t \eta(\tau)(1-e^{2ik(t-\tau)})m_l(\tau,k)d\tau \\ &= 1+I_1(t,k)+I_2(t,k)+I_3(t,k)+I_4(t,k) \end{aligned} \tag{4.113}$$

with $I_j : R\times C^+ \to C,\ 1\leq j\leq 4$ defined by the formulae

$$I_1(t,k) = \frac{1}{2ik}\int_0^t \eta(\tau)d\tau + \sum_{j=2}^{\gamma-1}\left(\frac{1}{2ik}\right)^j\int_0^t \eta(\tau)a_{j-1}(\tau)d\tau, \tag{4.114}$$

$$I_2(t,k) = -\frac{1}{2ik}\int_0^t \eta(\tau)(1-e^{2ik(t-\tau)})d\tau, \tag{4.115}$$

$$I_3(t,k) = -\sum_{s=2}^{\gamma-1}\left(\frac{1}{2ik}\right)^s\int_0^t \eta(\tau)a_{s-1}(\tau)e^{2ik(t-\tau)}d\tau \equiv -\sum_{s=2}^{\gamma-1}J_s(t,k), \tag{4.116}$$

$$I_4(t,k) = \frac{1}{2ik}\int_0^t \eta(\tau)a_\gamma(\tau)(1-e^{2ik(t-\tau)})d\tau. \tag{4.117}$$

Clearly, we only need to show that $I_j,\ 1\leq j\leq 4$ can be expressed in the form

$$\sum_{j=1}^{\gamma-1}\left(\frac{1}{2ik}\right)^j\alpha_j(t)+\left(\frac{1}{2ik}\right)^\gamma\alpha_\gamma(t,k) \tag{4.118}$$

with $\alpha_j : R\to R,\ 1\leq j\leq \gamma-1$ satisfying condition (4.110) and $\alpha_\gamma : R\times C^+\to C$ satisfying condition (4.111). Obviously, I_1 and I_4 are already in the form (4.118). We now use Lemma 3.3 to show that I_2, I_3 can also be expanded in the form (4.118). Observing that $\eta(t)=0$ for all $t\notin(0,T_1)$, $\eta^{(\gamma-2)}$ is absolutely continuous (see Lemma 3.9), and that $a_j^{(\gamma-j)}, 1\leq j\leq\gamma-1$ are absolutely continuous (due to the assumption of the induction), we can use formula (3.5) in Lemma 3.3 to expand I_2 and each term J_s $(s=1,\ldots,\gamma-1)$ of I_3 as

$$I_2(t,k) = \sum_{j=2}^{\gamma-1}\left(\frac{1}{2ik}\right)^j\eta^{(j-2)}(t)+\left(\frac{1}{2ik}\right)^\gamma b_1(t,k), \tag{4.119}$$

$$J_s(t,k) = \left(\frac{1}{2ik}\right)^s\int_0^t \eta(\tau)a_{s-1}(\tau)e^{2ik(t-\tau)}d\tau \tag{4.120}$$

$$= -\sum_{j=s+1}^{\gamma-1}\left(\frac{1}{2ik}\right)^j\frac{d^{(j-s-1)}}{dt^{(j-s-1)}}(\eta(\tau)a_{(s-1)}-\left(\frac{1}{2ik}\right)^\gamma b_s(t,k) \tag{4.121}$$

with $b_s : R\times C^+\to C$ uniformly bounded on $R\times C^+$ (see Lemma 3.3). Therefore, I_2 is in the form (4.118) due to (4.119), and I_3 is of the form (4.118) due to (4.121), (4.116). Thus, $m_{l+1}(t,k)$ can indeed be written in the form (4.109) satisfying conditions (4.110), (4.111). □

Corollary 4.11 *Suppose that for any $a \geq 0$, the region $K(a) \subset C$ is defined by the formulae*

$$K(a) = \{k | k \in C, Im(k) \geq 0, |k| \geq a\}. \tag{4.122}$$

Suppose further that the functions $m, n, m_\gamma, n_\gamma : R \times C^+ \to C$ are defined by the formulae (4.89), (4.90), (4.108) and

$$n_\gamma(t,k) = m_\gamma(t,k) - \frac{1}{2ik}\int_0^t \eta(\tau)e^{2ik(t-\tau)}m_\gamma(\tau,k)d\tau \tag{4.123}$$

respectively. Then under the conditions of the preceding lemma, there exist positive numbers A, c_1, c_2, c_3 such that

$$|m(t,k) - m_\gamma(t,k)| \leq \frac{c_1}{|k|^\gamma}, \tag{4.124}$$

$$|n(t,k) - n_\gamma(t,k)| \leq \frac{c_2}{|k|^\gamma} \tag{4.125}$$

for all $(t,k) \in R \times K(A)$, and

$$\left|\frac{n(t,k)}{m(t,k)} - 1\right| \leq \frac{c_3}{|k|^\gamma} \tag{4.126}$$

for all $(t,k) \in [T_1, \infty) \times K(A)$.

Proof. Due to (4.98), the norm of the integral operator F_k in (4.108) is of the order $O(|k|^{-1})$ for any $k \in C^+$, from which we observe that there exists $A > 0$, such that (4.124) is true.

Subtracting (4.123) from (4.90), we obtain

$$\begin{aligned} & n(t,k) - n_\gamma(t,k) \\ = \; & m(t,k) - m_\gamma(t,k) - \frac{1}{2ik}\int_0^t \eta(\tau)e^{2ik(t-\tau)}(m(\tau,k) - m_\gamma(\tau,k))d\tau \end{aligned} \tag{4.127}$$

Now, the estimate (4.125) is a direct consequence of (4.127), (4.124) and the fact that in (4.127), the expression

$$\frac{1}{2ik}\eta(\tau)e^{2ik(t-\tau)} \tag{4.128}$$

is uniformly bounded for all $k \in K(A)$, $-\infty < \tau \leq t < \infty$.

We now prove (4.126) by showing that there exists a positive number c_3 such that

$$\left|\frac{n_\gamma(t,k)}{m_\gamma(t,k)} - 1\right| \leq \frac{c_3}{|k|^\gamma} \tag{4.129}$$

for all $(t,k) \in [T_1,\infty) \times K(A)$. According to Lemma 4.10, $m_\gamma(t,k)$ can be expressed in the form

$$m_\gamma(t,k) = 1 + \sum_{j=1}^{\gamma-1} \left(\frac{1}{2ik}\right)^j a_j(t) + \left(\frac{1}{2ik}\right)^\gamma a_\gamma(t,k), \tag{4.130}$$

with $a_j, j = 1,\dots,\gamma$ satisfying conditions (4.110), (4.111). Therefore, we can assume that the constant A has been chosen such that for all $(t,k) \in R \times K(A)$,

$$|m_\gamma(t,k)| \geq \frac{1}{2}. \tag{4.131}$$

Combining (4.123) with (4.130), we obtain

$$n_\gamma(t,k) = m_\gamma(t,k) + I_2(t,k) + I_3(t,k) + I_5(t,k), \tag{4.132}$$

with $I_2, I_3(t,k)$ defined by (4.115), (4.116), and $I_5(t,k)$ defined by the formula

$$I_5(t,k) = \left(\frac{1}{2ik}\right)^{\gamma+1} \int_0^t \eta(\tau) a_\gamma(\tau,k) e^{2ik(t-\tau))} d\tau. \tag{4.133}$$

Noticing that $\eta(t) = 0$ for all $t \geq T_1$, we have

$$\begin{aligned} I_2(t,k) &= \left(\frac{1}{2ik}\right)^\gamma b_1(t,k), &(4.134)\\ J_s(t,k) &= \left(\frac{1}{2ik}\right)^\gamma b_s(t,k) &(4.135)\end{aligned}$$

for all $(t,k) \in [T_1,\infty) \times K(A)$, due to (4.119), (4.121). Consequently, there exists $c > 0$ such that

$$|I_2(t,k) + I_3(t,k) + I_5(t,k)| \leq \frac{c}{|k|^\gamma} \tag{4.136}$$

for all $(t,k) \in [T_1,\infty) \times K(A)$, since $a_\gamma(t,k)$, $b_s(t,k)$ are bounded for all $(t,k) \in [T_1,\infty) \times K(A)$, and $s = 1,\dots,\gamma-1$.

Now, (4.129) follows immediately from (4.132), (4.136) and (4.131). The estimate (4.126) is a direct consequence of (4.129), (4.124) and (4.125). □

Lemma 4.12 *Suppose that $q \in c_0^\gamma([0,1])$, $\gamma \geq 2$, $q^{(\gamma)}$ is absolutely continuous and $q(x) > -1$ for all $x \in R$. Then there exists a positive number c such that*

$$|p_-(x,k) - 1| \leq \frac{c}{|k|^\gamma} \tag{4.137}$$

for all $x \geq 1$, $k \in C^+$.

Proof. According to Corollary 3.11 and formula (3.41),

$$p_-(x,k) = \frac{\psi'_-(t,k)}{-ik\psi_-(t,k)} \tag{4.138}$$

for all $t \geq T_1$ (i.e., for all $x \geq 1$), $k \in C^+$. According to (4.89), (4.90) and (4.138)

$$p_-(x,k) = \frac{m(t,k)}{n(t,k)} \tag{4.139}$$

for all $t \geq T_1$, $k \in C^+$. Now, the lemma follows immediately from (4.139) and (4.126). □.

Remark 4.13 *By a similar calculation, one can show that under the conditions of the preceding lemma, there exist positive numbers $A > 0$, $c > 0$ such that*

$$|p_+(x,k) - 1| \leq \frac{c}{|k|^\gamma} \tag{4.140}$$

for all $x \leq 0$, $k \in C^+$.

Theorem 4.14 *Suppose that $q \in c_0^2([0,1])$, $q(x) > -1$ for all $x \in R$ and q'' is absolutely continuous. Suppose further that*

$$D = \{(x,k)|x \in R, Im(k) \geq 0\}. \tag{4.141}$$

Then
(a) ϕ_+ and ϕ_- are continuous functions of (x,k) and analytic functions of k for all $x \in R$ and $k \in C$;
(b) p_+ and p_- are continuous functions of (x,k) and analytic functions of k in D;
(c) there exists a positive number c such that for all $(x,k) \in D$

$$p_+(x,k) = \sqrt{1+q(x)} - \frac{q'(x)}{4(1+q(x))}\cdot\frac{1}{ik} + \epsilon_+(x,k), \tag{4.142}$$

$$p_-(x,k) = \sqrt{1+q(x)} + \frac{q'(x)}{4(1+q(x))}\cdot\frac{1}{ik} + \epsilon_-(x,k), \tag{4.143}$$

with $\epsilon_+, \epsilon_- : D \to C$ continuous functions such that

$$|\epsilon_+(x,k)| \leq \frac{c}{|k|^2}, \tag{4.144}$$

$$|\epsilon_-(x,k)| \leq \frac{c}{|k|^2}. \tag{4.145}$$

Proof. We only give the proof for ϕ_-, p_- since the proof for ϕ_+, p_+ is identical. We introduce two auxiliary functions ϕ and ϕ_1 via the formulae

$$\phi(x,k) = \phi_-(x,k), \tag{4.146}$$
$$\phi_1(x,k) = \phi_-'(x,k), \tag{4.147}$$

so that the equation (2.1) and the initial condition (2.5) for ϕ_- can be rewritten as a system of linear ODEs

$$\phi'(x,k) = \phi_1(x,k), \tag{4.148}$$
$$\phi_1'(x,k) = -k^2n^2(x)\phi(x,k), \tag{4.149}$$

subject to initial conditions

$$\phi(0,k) = 1, \tag{4.150}$$
$$\phi_1(0,k) = -ik. \tag{4.151}$$

According to Lemma 3.6, ϕ, ϕ_1 are continuous functions of (x,k) and entire functions of k for all $x \in R$ and $k \in C$, from which (a) follows immediately. Similarly, we obtain (b) by combining (a) with (2.16) and the fact that $\phi_-(x,k) \neq 0$ for all $(x,k) \in D$ (see Remark (4.3), Lemma 4.4 and Corollary 4.7).

The expansion (4.143) and the estimate (4.145) follow immediately from (3.41) (see Corollary 3.11 in Chapter 3), (4.83), (4.84), (4.87), and (4.88) (see Lemma 4.9). □

Corollary 4.15 *Denote by p p_+ or p_-. Then under the conditions of the preceding theorem, there exist positive number c_1, c_2 such that*

$$\left| e^{2ik\int_t^x p(\tau,k)d\tau} \right| \leq c_1, \tag{4.152}$$

for all $t, x \in [0,1]$, $k \in R$, or for all $0 \leq t \leq x \leq 1$, $k \in C^+$, and

$$|p'(x,k)| \leq c_2, \tag{4.153}$$

for all $x \in R$, $k \in C^+$.

Proof. Due to Statements (b), (c) of Theorem 4.14, the real part of the function

$$2ik\int_t^x p(\tau,k)d\tau \tag{4.154}$$

is uniformly bounded from above for $t, x \in [0,1]$, $k \in R$, or for all $0 \leq t \leq x \leq 1$, $k \in C^+$, from which (4.152) follows immediately. Estimate (4.153) is a direct consequence of Statement (c) of Theorem 4.14, and formulae (3.50), (3.51). □

Global upper and lower bounds for the impedance functions will be established in Theorem 4.17. We first obtain a partial result in the following lemma.

Lemma 4.16 *Suppose that for any positive numbers a, α, the domain $K(a,\alpha) \subset C$ is defined by the formula*

$$K(a,\alpha) = \{k | k \in C, Re(k) \in [-a,a], Im(k) \in [0,\alpha]\}. \tag{4.155}$$

Then under the conditions of the preceding theorem, for any $A > 0$, there exist positive numbers B, b, δ such that

$$\begin{aligned} |p_+(x,k)| &\leq B, & (4.156)\\ |p_-(x,k)| &\leq B, & (4.157)\\ Re(p_+(x,k)) &\geq b, & (4.158)\\ Re(p_-(x,k)) &\geq b, & (4.159) \end{aligned}$$

in the domain $R \times K(A,\delta)$.

Proof. Since the proof of (4.156), (4.158) is identical to that of (4.157), (4.159), we only provide the latter. Denoting by u, v the real and imaginary parts of p_- so that

$$p_-(x,k) = u(x,k) + iv(x,k), \tag{4.160}$$

the Riccati equation (3.51) for p_- can be rewritten in the form

$$\begin{aligned} u' &= -2kuv, & (4.161)\\ v' &= -k(v^2 - u^2 + n^2), & (4.162) \end{aligned}$$

for any $k \in R$. Integrating (4.161) on interval $[0,x]$ and observing that

$$u(x,k) = p_-(x,k) = 1 \tag{4.163}$$

for all $x \leq 0,\ k \in C$ (see (3.53)), we have

$$u(x,k) = e^{-2k\int_0^x v(t,k)dt} > 0 \tag{4.164}$$

for all $x, k \in R$. For any $A > 0$, $p_-, u = Re(p_-)$ are continuous functions of (x,k) in the compact domain $[0,1] \times K(A,\delta)$. Therefore, there exist positive numbers b_1, δ, B_1 such that

$$\begin{aligned} u(x,k) &\geq b_1 > 0 & (4.165)\\ |p_-(x,k)| &\leq B_1, & (4.166) \end{aligned}$$

for all $(x,k) \in [0,1] \times K(A,\delta)$, which proves the estimates (4.157), (4.159).

We now prove the estimates (4.157), (4.159) for all $x \geq 1$ using the formula

$$p_-(x,k) = \frac{1 - b_-^2(k) + i2b_-(k)\sin(kx - \alpha_-(k))}{1 + b_-^2(k) + 2b_-(k)\cos(kx - \alpha_-(k))}, \tag{4.167}$$

(see Remark (2.2)). According to Remark (2.2), $b(k) \geq 0$ is a real-valued continuous function of $k \in C$. We observe that

$$0 \leq b(k) < 1 \tag{4.168}$$

for all k in the close domain $K(A, \delta)$ since otherwise if $b(k) \geq 1$, the real part of $p_-(1, k)$

$$u(1,k) = \frac{1 - b_-^2(k)}{1 + b_-^2(k) + 2b_-(k)\cos(kx - \alpha_-(k))} \tag{4.169}$$

will be non-positive, contradicting (4.165). Due to (4.168), (4.167), there exist positive numbers b_2, B_2 such that

$$u(x,k) \geq b_2, \tag{4.170}$$

$$|p_-(x,k)| \leq B_2, \tag{4.171}$$

for all $x \geq 1$, $k \in K(A, \delta)$.

Now, (4.157), (4.159) follow immediately from (4.165), (4.166), (4.170), (4.171), and (4.163). □

Theorem 4.17 *Suppose that* $q \in c_0^2([0,1])$, $q(x) > -1$ *for all* $x \in R$ *and the second derivative of* q *is absolutely continuous. Then there exist real numbers* $B > 0$, $b > 0$ *such that*

$$|p_+(x,k)| \leq B, \tag{4.172}$$

$$|p_-(x,k)| \leq B, \tag{4.173}$$

$$Re(p_+(x,k)) \geq b, \tag{4.174}$$

$$Re(p_-(x,k)) \geq b, \tag{4.175}$$

in the domain

$$D = \{(x,k) | x \in R, Im(k) \geq 0\}. \tag{4.176}$$

Proof. Since the proof of (4.172), (4.174) is identical to that of (4.173), (4.175), we only provide the latter. According to the high-frequency asymptotics (4.143) in Theorem 4.14, there exist positive numbers A, b_1 such that

$$Re(p_-(x,k)) \geq b_1, \tag{4.177}$$

in the domain $D_1 \subset D$ defined by

$$D_1 = \{(x,k) | x \in R, |k| \geq A, Im(k) \geq 0\}. \tag{4.178}$$

Since $p_-(x,k)$ is a continuous function of $(x,k) \in D_1$, there exists a positive number B_1 such that

$$|p_-(x,k)| \leq B_1, \tag{4.179}$$

for all $(x, k) \in D_1$. For such a number $A > 0$, according to Lemma 4.16, there exist positive numbers δ, B_2, b_2 such that

$$\begin{aligned} |p_-(x,k)| &\leq B_2, & (4.180) \\ Re(p_-(x,k)) &\geq b_2, & (4.181) \end{aligned}$$

in the domain $D_2 \subset D$ defined by the formula

$$D_2 = \{(x,k)|x \in R, Re(k) \in [-A, A], Im(k) \in [0, \delta]\}. \tag{4.182}$$

Now, according to Lemmas 4.5, 4.6, there exist positive numbers B_3, b_3 such that

$$\begin{aligned} |p_-(x,k)| &\leq B_3, & (4.183) \\ Re(p_-(x,k)) &\geq b_3, & (4.184) \end{aligned}$$

in the domain $D_3 \subset D$ defined by

$$D_3 = \{(x,k)|x \in R, Re(k) \in [-A, A], Im(k) \geq \delta\}. \tag{4.185}$$

The estimates (4.173), (4.175) for $(x, k) \in D$ follow immediately from the estimates for $(x, k) \in D_1$, D_2, D_3 since $D = D_1 \cup D_2 \cup D_3$. $\square$

The following theorem furnishes the analytical apparatus for the error analysis of the truncated trace formula (see (4.198)).

Theorem 4.18 *Suppose that $q \in c_0^m([0,1])$, $m \geq 2$, $q^{(m)}$ is absolutely continuous and $q(x) > -1$ for all $x \in R$. Then there exists a positive number a such that*

$$\left|\overline{p_+(x,k)} - p_-(x,k)\right| \leq \frac{a}{|k|^m} \tag{4.186}$$

for all $(x, k) \in R \times C^+$.

Proof. According to Lemma 4.12 and Remark (4.13), (4.186) is true for all $x \notin (0, 1)$. In order to prove the theorem for $x \in (0, 1)$, we observe that $\overline{p_+}$ and p_- obey the same Riccati equation (3.51) due to (3.50), (3.51). The difference, $s = \overline{p_+} - p_-$, satisfies the ODE

$$s'(x,k) = ik\left(\overline{p_+} + p_-\right)s \tag{4.187}$$

with the solution

$$s(x,k) = e^{-ik\int_0^x \left(\overline{p_+(t,k)} + p_-(t,k)\right)dt} s(0,k). \tag{4.188}$$

Corollary 4.15 indicates that there exists constant $b > 0$ such that

$$\left| e^{-ik\int_0^x (\overline{p_+(t,k)}+p_-(t,k))dt} \right|, \tag{4.189}$$

for all $(x, k) \in [0, 1] \times R$. Due to Remark (4.13), there exists a positive number c such that for all $k \in R$,

$$|s(0,k)| = |p_+(0,k) - p_-(0,k)| = |p_+(0,k) - 1| \leq \frac{c}{|k|^m}. \tag{4.190}$$

Now, (4.186) for $x \in (0, 1)$ follows immediately from (4.188), (4.189), (4.190). □

4.3 Trace Formulae

In this section, we prove Theorem 4.19, which is both the purpose of this chapter, and the principal analytical tool of this thesis. Theorem 4.19 describes the so-called trace formulae for the impedance functions p_+, p_- (for a more detailed discussion of the term "trace formulae", see, for example, [7]). In fact, only the formula (4.194) is to be used by the reconstruction algorithm of the following chapter. We present the formulae (4.191), (4.192), (4.193) for completeness, since some of them appear to be well-known, and attempts have been made to use them in reconstruction algorithms (see, for example, [8]). See also Section 5.1 below for a more detailed discussion of the use of trace formulae in reconstruction schemes

Theorem 4.19 *(Trace formulae) Suppose that $q \in c_0^m([0,1])$, $m \geq 2$, $q^{(m)}$ is absolutely continuous and $q(x) > -1$ for all $x \in R$. Then*
(a)

$$\sqrt{1 + q(x)} = \lim_{a \to +\infty} \frac{1}{2a} \int_{-a}^{a} p_+(x,k)dk. \tag{4.191}$$

(b)

$$q'(x) = \lim_{a \to +\infty} \frac{2}{ia}(1 + q(x)) \int_{-a}^{a} k \cdot p_+(x,k)dk. \tag{4.192}$$

(c)

$$\sqrt{1 + q(x)} = \lim_{a \to +\infty} \frac{1}{4a} \int_{-a}^{a} (p_+(x,k) + p_-(x,k))dk. \tag{4.193}$$

(d)

$$q'(x) = \frac{2}{\pi}(1 + q(x)) \int_{-\infty}^{\infty} (p_+(x,k) - p_-(x,k))dk. \tag{4.194}$$

Morc precisely, there exist positive numbers c_1, c_2, c_3, c_4 such that

$$\left|\sqrt{1+q(x)} - \frac{1}{2a}\int_{-a}^{a} p_+(x,k)dk\right| \leq \frac{c_1}{a}, \tag{4.195}$$

$$\left|q'(x) - \frac{2}{ia}(1+q(x))\int_{-a}^{a} k\cdot p_+(x,k)dk\right| \leq \frac{c_2}{a}, \tag{4.196}$$

$$\left|\sqrt{1+q(x)} - \frac{1}{4a}\int_{-a}^{a}(p_+(x,k)+p_-(x,k))dk\right| \leq \frac{c_3}{a^2}, \tag{4.197}$$

$$\left|q'(x) - \frac{2}{\pi}(1+q(x))\int_{-a}^{a}(p_+(x,k)-p_-(x,k))dk\right| \leq \frac{c_4}{a^{(m-1)}}. \tag{4.198}$$

for all $x \in R$.

Proof. Since the proofs of trace formulae (a),(b),(c), and (d) are similar, we only present that of (d). According to statement (c) of Theorem 4.14, there exists $c > 0$ such that

$$\left|(p_+(x,k)-p_-(x,k)) - \left(-\frac{q'(x)}{2(1+q(x))}\frac{1}{ik}\right)\right| \leq \frac{c}{|k|^2}. \tag{4.199}$$

for all $(x,k) \in R \times C^+$. Denoting by Γ the upper half circle of radius A, with clockwise orientation, in the complex k-plane, i.e.,

$$\Gamma = \{k | k \in C^+,\ |k| = A\}, \tag{4.200}$$

and noting that $p_+ - p_-$ is an analytic function of $k \in C^+$, we obtain

$$\int_{-A}^{A}(p_+(x,k)-p_-(x,k))dk = \int_{\Gamma}(p_+(x,k)-p_-(x,k))dk. \tag{4.201}$$

Substituting (4.199) into (4.201), we have

$$\int_{-A}^{A}(p_+(x,k)-p_-(x,k))dk = \frac{\pi q'(x)}{2(1+q(x))} + O(k^{-1}) \tag{4.202}$$

from which (4.194) follows immediately.

In order to prove the estimate (4.198), we rewrite (4.194) as

$$q'(x) = \frac{2}{\pi}(1+q(x))\int_{-a}^{a}(p_+(x,k)-p_-(x,k))dk + I(a) \tag{4.203}$$

with $I(a)$ given by the formula

$$I(a) = \frac{2}{\pi}(1+q(x))\left(\int_{-\infty}^{-a} + \int_{a}^{\infty}\right)(p_+(x,k)-p_-(x,k))dk. \tag{4.204}$$

Now, formula (4.74) implies

$$I(a) = \frac{2}{\pi}(1 + q(x)) \left(\int_{-\infty}^{-a} + \int_{a}^{\infty} \right) \left(\overline{p_+(x,k)} - p_-(x,k) \right) dk, \tag{4.205}$$

and according to (4.186), there exists a constant c_4 such that

$$|I(a)| \leq \frac{c_4}{|k|^{(m-1)}}, \tag{4.206}$$

from which (4.198) follows immediately. □

Chapter 5

The Reconstruction Algorithm

5.1 Reconstruction via trace formulae–an informal description

An examination of the formulae (4.191)- (4.194) in combination with the Riccati equations (3.50), (3.51) immediately suggests an algorithm for the reconstruction of the parameter q given the impedance function $p_+(x_0, k)$ measured at some point $x_0 \in R$ outside the scatterer. Namely, one is tempted to substitute one of the formulae (4.191)- (4.194) (for example, (4.191)) into (3.50), obtaining

$$p'_+(x,k) = -ik\left(p_+^2(x,k) - \lim_{a\to}\left(\frac{1}{2a}\int_{-a}^{a} p_+(x,k)dk\right)^2\right), \tag{5.1}$$

and attempt to view (5.1) as a differential equation for the function $p : R^1 \times R^1 \rightarrow C$.

Needless to say, standard existence and uniqueness theorems are not applicable to 'differential equations' of the form (5.1). Furthermore, in order to be numerically useful, the integral in (5.1) would have to be replaced with some finite quadrature formulae. The latter procedure is significantly complicated by the fact that the function p_+ is defined on the whole real line, and its domain of definition has to be truncated before discretization. It turns out that the solution of (5.1) is not unique, except in a very carefully chosen class of functions p. Such a class of functions has been successfully specified (see, for example, [8]). The resulting numerical scheme is, however, quite expensive, and the construction is not rigorous, though we believe that this could be made so. The same problem arises if one attempts to use the trace formulae (4.192), (4.193), and the conceptual reason for this situation is summarized in the following observation.

An immediate consequence of the formula (4.191) is

$$\sqrt{1+q(x)} = \lim_{a\to+\infty} \frac{1}{2a} \cdot \left(\int_{-a}^{-b} p_+(x,k)dk + \int_b^a p_+(x,k)dk \right), \tag{5.2}$$

for any positive real b. Thus, the 'differential equation' (5.1) can be replaced with

$$p'_+(x,k) = -ik\left(p_+^2(x,k) - \left(\lim_{a\to+\infty} \frac{1}{2a} \left(\int_{-a}^{-b} p_+(x,k)dk + \int_b^a p_+(x,k)dk \right) \right)^2 \right) \tag{5.3}$$

and a convergence, uniqueness, etc. proof valid for (5.1) would also be valid for (5.3), unless some extremely subtle phenomenon interfered.

However, given a smooth scatterer q, for any $\varepsilon > 0$, one can choose a sufficiently large b that

$$\left| \sqrt{1+q(x)} - p_+(x,k) \right| < \varepsilon \tag{5.4}$$

for any $k \geq b$. If the scattered data $p_+(x_0,k)$ have been collected at some point x_0 outside a smooth scatterer, (5.4) assumes the form

$$|1 - p_+(x,k)| < \varepsilon. \tag{5.5}$$

In other words, a reconstruction algorithm using the 'differential equation' (5.3) with a sufficiently large b would effectively reconstruct the parameter $q(x)$ for all $x \in [0,1]$ from a single measurement, the latter being equal to 1 (!). Another way to make this observation is to notice that the formula (4.191) is simply the WKB approximation to the impedance function p_+, and that in the WKB regime, the back-scattered field is absent. A similar problem arises if one attempts to combine formulae (4.192), (4.193) with (3.50), and view the result as a "system of ordinary differential equations".

In the case of a discontinuous scatterer q, the WKB expansions (4.142), (4.143) are invalid. On the other hand, the trace formulae (4.191), (4.194) are valid (if the limits in these formulae are interpreted properly), and can be combined with the equations (3.50), (3.51) to obtain a numerical scheme for detecting discontinuities in the scatterer. If q is piece-wise constant, such a scheme will reconstruct it effectively, and time-domain versions of this procedure are known as layer-stripping algorithms (see, for example, [12], [13], [14]).

While the author failed to find the trace formulae (4.192), (4.193) in the literature, they appear to be well-known among specialists, being an immediate consequence of the WKB analysis of the equation (3.50). On the other hand, the formula (4.194) does appear to be new, and its combination with the equation (3.50) immediately leads to a robust reconstruction algorithm. While we postpone a detailed construction and analysis of such a scheme till Section 5.2, in

the following observation we summarize the conceptual reasons for its analytical and numerical effectiveness.

Formula (4.198) means that approximating the trace formula (4.194) with its 'truncated' version

$$q'(x) \sim \frac{2}{\pi}(1+q(x)) \int_{-a}^{a} (p_+(x,k) - p_-(x,k))dk, \tag{5.6}$$

we make an error of the order $a^{-(m-1)}$, where m is the smoothness of the scatterer. Thus, for a sufficiently smooth scatterer and a sufficiently large a, (5.6) is an extremely good approximation to the trace formula (4.194).

Now, for the system of equations (3.50), (3.51), (5.6), it is not hard to prove existence, uniqueness, etc. theorems of the type valid for systems of ODEs (since now for a fixed value of x, the functions $p_+(x,k), p_-(x,k) : [-a,a] \to C$ are defined on a compact interval, as opposed to the whole line). The remainder of this thesis is devoted largely to proving such facts (see Theorem 5.1 below), and to a numerical implementation of the resulting procedure. The latter is also quite straightforward, since it only involves constructing a quadrature formula for the evaluation of the integral in (4.194), where it is taken over an interval of finite length. Furthermore, for all practical purposes, the integrand vanishes at the ends of the domain of integration together with all its derivatives, completely obviating the issue of the choice of the quadrature formula, and leading to extremely accurate numerical procedures (see Remark 6.3 below).

5.2 Reconstruction via trace formulae–a formal description

Now, we are prepared to construct a system of integro-differential equations whose initial conditions are the values of the impedance functions p_+, p_- measured outside the scatterer, and whose solution reconstructs the potential q for all $x \in [0,1]$. We will consider a system of integro-differential equations

$$\begin{aligned} p'_{a+}(x,k) &= -ik(p^2_{a+}(x,k) - (1+q_a(x))), && (5.7)\\ p'_{a-}(x,k) &= ik(p^2_{a-}(x,k) - (1+q_a(x))), && (5.8)\\ q'_a(x) &= \frac{2}{\pi}(1+q_a(x)) \int_{-a}^{a} (p_{a+}(x,z) - p_{a-}(x,z))dz, && (5.9) \end{aligned}$$

with respect to the functions $p_{a+}, p_{a-} : [0,1] \times [-a,a] \to C$, $q_a : [0,1] \to R$, subject to the initial conditions

$$\begin{aligned} p_{a+}(0,k) &= p_0(k), && (5.10)\\ p_{a-}(0,k) &= 1, && (5.11)\\ q(0) &= 0. && (5.12) \end{aligned}$$

It turns out that for sufficiently large a, the system (5.7)–(5.12)has a unique solution for all $x \in [0,1]$, that this solution is stable with respect to small perturbations of the initial data $p_0(k)$, and that q_a converges to q as $a \to \infty$. The following theorem and Lemmas 5.2–5.4 formalize these facts.

Theorem 5.1 *(Convergence of the inversion algorithm) Suppose that $q \in c_0^m([0,1])$ $m \geq 4$, $q^{(m)}$ is absolutely continuous and $q(x) > -1$ for all $x \in R$. Then there exist constants $A > 0, c > 0$ such that*

$$|q(x) - q_a(x)| \leq \frac{c}{a^{(m-1)}} \tag{5.13}$$

for all $x \in [0,1]$, $a \geq A$.

Since the proof of this theorem is quite involved, we break its technical part into three lemmas which are then directly used in the proof of Theorem 5.1.

Lemma 5.2 *Suppose that $q \in c_0^m([0,1])$, $m \geq 4$, $q^{(m)}$ is absolutely continuous and $q(x) > -1$ for all $x \in R$. Suppose further that the function space Σ is defined by the formula*

$$\Sigma = \{[\alpha,\beta,\gamma] | \alpha,\beta \in c([0,1] \times [-a,a]), \gamma \in c([0,1])\}, \tag{5.14}$$

equipped with the norm

$$\|f\| = \max(\|\alpha\|, \|\beta\|, \|\gamma\|), \tag{5.15}$$

with $f = [\alpha,\beta,\gamma] \in \Sigma$. Finally, suppose that for any $a > 0$, the functions $f_a, w, \epsilon_a : R \to R$ are defined by the formulae

$$\begin{aligned} f_a(x) &= \frac{2}{\pi}\int_{-a}^{a}(p_+(x,k) - p_-(x,k))dk, & (5.16)\\ w(x) &= \frac{2}{\pi}(1+q(x)), & (5.17)\\ \epsilon_a(x) &= -w(x)\left(\int_{-\infty}^{-a} + \int_a^{\infty}\right)(p_+(x,k) - p_-(x,k))dk. & (5.18) \end{aligned}$$

Then the error function $u = [e_+, e_-, h] \in \Sigma$ defined by the formulae

$$\begin{aligned} e_+(x,k) &= p_{a+}(x,k) - p_+(x,k), & (5.19)\\ e_-(x,k) &= p_{a-}(x,k) - p_-(x,k), & (5.20)\\ h(x) &= q_a(x) - q(x) & (5.21) \end{aligned}$$

satisfies the equation

$$L(u)(x,k) = N(u)(t,k) + [0,0,\epsilon_a(t)], \tag{5.22}$$

where $L, N : \Sigma \to \Sigma$ are defined by the formulae

$$L(u) = \begin{bmatrix} e_+(x,k) - ik\int_0^x h(t)e^{-2ik\int_t^x p_+(\tau,k)d\tau}dt \\ e_-(x,k) + ik\int_0^x h(t)e^{2ik\int_t^x p_-(\tau,k)d\tau}dt \\ h(x) - \int_0^x \left(h(t)f_a(t) + w(t)\int_{-a}^a (e_+ - e_-)(t,z)dz\right)dt \end{bmatrix} \quad (5.23)$$

$$N(u) = \begin{bmatrix} -ik\int_0^x e_+^2(t,k)e^{-2ik\int_t^x p_+(\tau,k)d\tau}dt \\ ik\int_0^x e_-^2(t,k)e^{2ik\int_t^x p_-(\tau,k)d\tau}dt \\ \frac{2}{\pi}\int_0^x h(t)\int_{-a}^a (e_+(t,z) - e_-(t,z))dzdt \end{bmatrix}. \quad (5.24)$$

Proof. We know that the functions p_+, p_-, q satisfy the ODEs

$$p'_+(x,k) = -ik(p_+^2(x,k) - (1+q(x)), \quad (5.25)$$
$$p'_-(x,k) = ik(p_-^2(x,k) - (1+q(x)), \quad (5.26)$$
$$q'(x) = \frac{2}{\pi}(1+q(x))\int_{-\infty}^{\infty}(p_+(x,k) - p_-(x,k))dk, \quad (5.27)$$

for all $x \in R$, any $k \in C^+$, and that the functions p_{a+}, p_{a-}, q_a satisfy the ODEs

$$p'_{a+}(x,k) = -ik(p_{a+}^2(x,k) - (1+q_a(x))), \quad (5.28)$$
$$p'_{a-}(x,k) = ik(p_{a-}^2(x,k) - (1+q_a(x))), \quad (5.29)$$
$$q'_a(x) = \frac{2}{\pi}(1+q_a(x))\int_{-a}^{a}(p_{a+}(x,z) - p_{a-}(x,z))dz. \quad (5.30)$$

for all $(x,k) \in [0,1] \times [-a,a]$, subject to initial conditions

$$p_{a+}(0,k) = p_+(0,k), \quad (5.31)$$
$$p_{a-}(0,k) = p_-(0,k) = 1, \quad (5.32)$$
$$q_a(0) = q(0) = 0. \quad (5.33)$$

for all $k \in [-a,a]$. Subtracting equations (5.25), (5.26), (5.27) from equations (5.28), (5.29), (5.30) respectively, we observe that $[e_+, e_-, h]$ (see (5.19), (5.20), (5.21)) satisfies the ODEs

$$e'_+(x,k) = -ik\left(2p_+(x,k)e_+(x,k) + e_+^2(x,k) - h(x)\right), \quad (5.34)$$
$$e'_-(x,k) = ik\left(2p_-(x,k)e_-(x,k) + e_-^2(x,k) - h(x)\right), \quad (5.35)$$
$$h'(x) = h(x)f_a(x) + w(x)\int_{-a}^{a}(e_+(x,z) - e_-(x,z))dz$$
$$+\frac{2}{\pi}h(x)\int_{-a}^{a}(e_+(x,z) - e_-(x,z))dz + \epsilon_a(x), \quad (5.36)$$

subject to the initial conditions

$$e_+(0,k) = e_-(0,k) = h(0) = 0. \quad (5.37)$$

We now convert the initial value problem (5.28)-(5.33) as a system of integral equations. Multiplying (5.34) by the function

$$e^{2ik\int_0^x p_+(t,k)dt}, \tag{5.38}$$

we have

$$\frac{d}{dx}\left(e^{2ik\int_0^x p_+(t,k)dt}e_+(x,k)\right) = -ik\cdot e^{2ik\int_0^x p_+(t,k)dt}\left(e_+^2(x,k)-h(x)\right). \tag{5.39}$$

Integrating the result over the interval $[0,x]$, we obtain

$$e_+(x,k)-ik\int_0^x h(t)e^{-2ik\int_t^x p_+(\tau,k)d\tau}dt = -ik\int_0^x e_+^2(t,k)e^{-2ik\int_t^x p_+(\tau,k)d\tau}dt. \tag{5.40}$$

A similar calculation reduces (5.35) to the equation

$$e_-(x,k)+ik\int_0^x h(t)e^{2ik\int_t^x p_-(\tau,k)d\tau}dt = ik\int_0^x e_-^2(t,k)e^{2ik\int_t^x p_-(\tau,k)d\tau}dt. \tag{5.41}$$

An integration of (5.36) over the interval $[0,x]$ converts (5.36) into the integral equation

$$\begin{aligned} & h(x)-\int_0^x h(t)f_a(t)dt-\int_0^x w(t)\int_{-a}^a(e_+(t,z)-e_-(t,z))dzdt \\ = & \ \frac{2}{\pi}\int_0^x h(t)\int_{-a}^a(e_+(t,z)-e_-(t,z)dzdt+\int_0^x \epsilon_a(t)dt. \end{aligned} \tag{5.42}$$

Clearly, equations (5.40), (5.41), (5.42) is equivalent to (5.22), which completes the proof. □

Lemma 5.3 *Under the conditions of Lemma 5.2, there exists a positive number c_1 such that for any $f,g\in\Sigma$, there exist continuous functions $\delta_1,\delta_2:[0,1]\times[-a,a]\to C$, $\delta_3:[0,1]\to C$ such that*

$$N(f)(x,k)-N(g)(x,k)=[\delta_1(x,k),\delta_2(x,k),\int_0^x\delta_3(t)dt], \tag{5.43}$$

and

$$\max(\|\delta_1\|,\|\delta_2\|,\|\delta_3\|)\le c_1\cdot a\cdot\max(\|f\|,\|g\|)\,\|f-g\|. \tag{5.44}$$

Proof. Formula (5.43) is a direct consequence of (5.24). In fact, we have

$$\delta_1(x,k) = -ik\int_0^x(f_1^2(t,k)-g_1^2(t,k))e^{-2ik\int_t^x p_+(\tau,k)d\tau}dt, \tag{5.45}$$

$$\delta_2(x,k) = ik\int_0^x(f_2^2(t,k)-g_2^2(t,k))e^{2ik\int_t^x p_-(\tau,k)d\tau}dt, \tag{5.46}$$

$$\delta_3(x) = \frac{2}{\pi}\int_{-a}^a\{f_3(x)(f_1-f_2)(x,z)-g_3(x)(g_1-g_2)(x,z)\}dz \tag{5.47}$$

for any $f = [f_1, f_2, f_3] \in \Sigma$, $g = [g_1, g_2, g_3] \in \Sigma$. In order to prove (5.44), we first observe that due to Corollary 4.15, there exists a positive number c_4 such that

$$\begin{aligned} \left| e^{-2ik\int_t^x p_+(\tau,k)d\tau} \right| &\leq c_4, & (5.48) \\ \left| e^{2ik\int_t^x p_-(\tau,k)d\tau} \right| &\leq c_4, & (5.49) \end{aligned}$$

for all $t, x \in [0,1]$, $k \in R$. Observing that $|k| \leq a$, $0 \leq x \leq 1$, and using the estimate (5.48), we obtain the estimate

$$\|\delta_1\| \leq a \cdot c_4 \|f + g\| \cdot \|f - g\|. \tag{5.50}$$

A similar calculation shows that

$$\|\delta_2\| \leq a \cdot c_4 \|f + g\| \cdot \|f - g\|, \tag{5.51}$$

and we obtain the estimate for δ_3 by first regrouping (5.47):

$$\begin{aligned} \|\delta_3\| &= \frac{2}{\pi} \sup_{x\in[0,1]} \Big| \Big((f_3(t) - g_3(t)) \int_{-a}^{a} (f_1(t,z) - f_2(t,z)) dz \\ &\quad + g_3(t) \int_{-a}^{a} ((f_1(t,z) - g_1(t,z)) - (f_2(t,z) - g_2(t,z))) dz \Big) \Big| \\ &\leq \frac{2}{\pi} \left(\|f - g\| \int_{-a}^{a} \|f + g\| dz + \|g\| \int_{-a}^{a} 2\|f - g\| dz \right) \\ &\leq a \cdot \frac{4}{\pi} \|f - g\| \left(\|f + g\| + 2\|g\| \right) \qquad (5.52) \end{aligned}$$

Now, (5.44) follows immediately from (5.50), (5.51), (5.52). □

Lemma 5.4 *Under the conditions of Lemma 5.2, there exist positive numbers c_2, c_3 such that for any $\delta \in \Sigma$ of the form*

$$\delta(x,k) = [\delta_1(x,k), \delta_2(x,k), \int_0^x \delta_3(t)dt], \tag{5.53}$$

the linear equation

$$L(v) = \delta \tag{5.54}$$

has a unique solution $v = [v_1, v_2, v_3] \in \Sigma$. Furthermore,

$$\|v\| \leq c_2 \cdot a \max(\|\delta_1\|, \|\delta_2\|) + c_3 \|\delta_3\|. \tag{5.55}$$

Proof. We only need to prove (5.55), since the existence and uniqueness of the solution v of the linear equation (5.54) is a direct consequence of the estimate

(5.55). Due to (5.23), (5.53), the equation (5.54) can be rewritten in the form

$$v_1(x,k) = ik\int_0^x v_3(t)e^{-2ik\int_t^x p_+(\tau,k)d\tau}dt + \delta_1(x,k), \tag{5.56}$$

$$v_2(x,k) = -ik\int_0^x v_3(t)e^{2ik\int_t^x p_-(\tau,k)d\tau}dt + \delta_2(x,k) \tag{5.57}$$

$$\begin{aligned} v_3(x) &= \int_0^x v_3(t)f_a(t)dt + \int_0^x w(t)\int_{-a}^a(v_1(t,z) - v_2(t,z)dzdt \\ &\quad + \int_0^x \delta_3(t)dt. \end{aligned} \tag{5.58}$$

In order to prove (5.55), we first eliminate v_1, v_2 from (5.58) and obtain an estimate for v_3. Subtracting (5.57) from (5.56), and integrating the result over the interval $[-a,a]$, we obtain

$$\begin{aligned} &\int_{-a}^a (v_1(x,z) - v_2(x,z))\,dz \\ &= \int_0^x v_3(t)\int_{-a}^a iz\left(e^{-2iz\int_t^x p_+(\tau,z)d\tau} + e^{2iz\int_t^x p_-(\tau,z)d\tau}\right)dzdt \\ &\quad + \int_{-a}^a(\delta_1(x,z) - \delta_2(x,z))dz \\ &= \int_0^x g_a(x,t)v_3(t)dt + 4a\cdot s_a(x), \end{aligned} \tag{5.59}$$

with $g_a : [0,1]\times[0,1] \to C$, $s_a : [0,1] \to C$ given by the formulae

$$g_a(x,t) = \int_{-a}^a iz\left(e^{2iz\int_t^x p_+(\tau,z)d\tau} + e^{2iz\int_t^x p_-(\tau,z)d\tau}\right)dz, \tag{5.60}$$

$$s_a(x) = \frac{1}{4a}\int_{-a}^a(\delta_1(x,z) - \delta_2(x,z))dz. \tag{5.61}$$

Combining (5.58) with (5.59), we obtain

$$\begin{aligned} v_3(x) &= \int_0^x v_3(t)f_a(t)dt + \int_0^x w(t)\int_0^t g_a(t,\tau)v_3(\tau)d\tau dt \\ &\quad + 4a\int_0^x w(t)s_a(t)dt + \int_0^x \delta_3(t)dt. \end{aligned} \tag{5.62}$$

We will obtain the estimate (5.72) for v_3 (see below) by first proving (5.63), (5.64), (5.65), and (5.69) for functions f_a, w, g_a, s_a. Obviously, there exist constants $c_5 > 0, c_6 > 0$ such that

$$|w(x)| \le c_5 \tag{5.63}$$

for all $x \in R$ due to (5.17), and

$$|f_a(x)| \le c_6 \tag{5.64}$$

for all $x \in [0,1]$, any $a > 0$, due to (5.16), (4.198), and

$$|s_a(x)| \leq \max(\|\delta_1\|, \|\delta_2\|). \tag{5.65}$$

due to (5.61). Observing that

$$\int_{-a}^{a} z \cdot e^{-2iz\int_t^x p_+(\tau,z)d\tau} dz = -\int_{-a}^{a} z \cdot e^{2iz\int_t^x \overline{p_+(\tau,z)}d\tau} dz \tag{5.66}$$

due to (4.72), and combining (5.60) with (5.66), we have

$$g_a(x,t) = \int_{-a}^{a} iz\left(e^{2iz\int_t^x p_-(\tau,z)d\tau} - e^{2iz\int_t^x \overline{p_+(\tau,z)}d\tau}\right) dz. \tag{5.67}$$

According to Theorem 4.18, for any $x \in R$, the function

$$p_-(x,k) - \overline{p_+(x,k)} \tag{5.68}$$

decays uniformly like k^{-m}, for $k \in R$, and consequently, the integrand in (5.67) decays like $k^{-(m-2)}$ uniformly with respect to $t, x \in [0,1]$. Since we have assumed that $m \geq 4$, there exists a constant $c_7 > 0$ such that

$$|g_a(x,t)| \leq c_7, \tag{5.69}$$

for all $t, x \in [0,1]$, $a > 0$. Now, combining the integral equation (5.62) with the estimates (5.63), (5.64), (5.65), (5.69), we have

$$\begin{aligned} |v_3(x)| &\leq c_6\int_0^x |v_3(t)|dt + c_5 \cdot c_7 \int_0^x \int_0^t |v_3(\tau)|dt d\tau \\ &\quad +4a \cdot c_5 \cdot x \max(\|\delta_1\|, \|\delta_2\|) + \|\delta_3\| \\ &\leq \int_0^x (c_6 + c_5c_7)|v_3(t)|dt + 4a \cdot c_5 x \max(\|\delta_1\|, \|\delta_2\|) + \|\delta_3\| \end{aligned} \tag{5.70}$$

Now, the estimate for v_3 follows from Gronwall's inequality (see Lemma 3.5),

$$\begin{aligned} |v_3(x)| &\leq 4a \cdot c_5 \cdot x \max(\|\delta_1\|, \|\delta_2\|) + \|\delta_3\| \\ &+ c_8\int_0^x (4a \cdot c_5 t \max(\|\delta_1\|, \|\delta_2\|) + \|\delta_3\|)\, e^{(x-t)(c_6+c_5c_7)}dt, \end{aligned} \tag{5.71}$$

with $c_8 = c_6 + c_5 \cdot c_7$. Clearly, there exist positive numbers c_9, c_{10} such that

$$|v_3(x)| \leq c_9 \max(\|\delta_1\|, \|\delta_2\|) + c_{10}\|\delta_3\|, \tag{5.72}$$

for all $x \in [0,1]$, we thus have the estimate for v_3 (see (5.55)).

In order to obtain similar estimates for v_1, v_2, we first provide an estimate for the derivative of v_3. Differentiating (5.62), we have

$$v_3'(x) = v_3(x)f_a(x)dt + w(x)\int_0^x g_a(x,t)v_3(t)dt + 4a \cdot w(x)s_a(x) + \delta_3(x). \tag{5.73}$$

Combining (5.73) with (5.72), we observe that there exist positive numbers c_{11}, c_{12} such that

$$|v_3'(x)| \le c_{11} \max(\|\delta_1\|, \|\delta_2\|) + c_{12}\|\delta_3\|. \tag{5.74}$$

Integrating by parts in (5.56) yields

$$\begin{aligned} v_1(x,k) &= \frac{1}{2}\int_0^x \frac{v_3(t)}{p_+(t,k)} d\left(e^{-2ik\int_t^x p_+(\tau,k)d\tau}\right) + \delta_1(x,k) \\ &= \delta_1(x,k) + \frac{1}{2}\left(\frac{v_3(x)}{p_+(x,k)}\right. \\ &\quad \left. - \int_0^x \frac{v_3'(t)p_+(t,k) - v_3(t)p_+'(t,k)}{p_+^2(t,k)} e^{-2ik\int_t^x p_+(\tau,k)d\tau} dt\right). \end{aligned} \tag{5.75}$$

For all $(x,k) \in R \times C^+$, p_+ is uniformly bounded, $Re(p_+)$ is uniformly bounded from below by a positive number (see Theorem 4.17). Due to Corollary 4.15, p_+' and

$$e^{-2ik\int_t^x p_+(\tau,k)d\tau} \tag{5.76}$$

are uniformly bounded for all $x, t \in [0,1]$, $k \in R$. Therefore, combining (5.75) with (5.72), (5.74), (4.152), we observe that there exist positive numbers c_{13}, c_{14} such that

$$|v_1(x,k)| \le c_{13} \max(\|\delta_1\|, \|\delta_2\|) + c_{14}\|\delta_3\|, \tag{5.77}$$

and a similar calculation shows that

$$|v_2(x,k)| \le c_{13} \max(\|\delta_1\|, \|\delta_2\|) + c_{14}\|\delta_3\| \tag{5.78}$$

for all $x \in [0,1]$, $k \in [-a,a]$. Now, the estimate (5.55) follows immediately from (5.72), (5.77), (5.78). □

Using Lemmas 5.2, 5.3, 5.4, we now proceed with the proof of Theorem 5.1.

Proof of Theorem 5.1. Theorem 4.19 implies that there exists positive numbers b_1, b_2 such that

$$|f_a(x)| \le b_1, \tag{5.79}$$

$$|\epsilon_a(x)| \le \frac{b_2}{a^{(m-1)}}. \tag{5.80}$$

We prove the theorem by showing that there exist positive numbers A, c such that for all $a \ge A$, the solution $u = [e_+, e_-, h] \in \Sigma$ exists (see Lemma 5.2 for the definitions of u, Σ), and that

$$\|u\| \le \frac{c}{a^{(m-1)}}. \tag{5.81}$$

We will obtain the solution u of the equation (5.22) via the following iterative procedure:

$$\begin{aligned} u_0 &= 0, && (5.82)\\ L(u_{n+1}) &= N(u_n) + [0, 0, \epsilon_a(t)], && (5.83) \end{aligned}$$

with L, N defined by the formulae (5.23), (5.24), respectively. Clearly, we only need to show that there exist positive numbers A, c such that for all $a \geq A$

$$\|u_n\| \leq \frac{c}{a^{(m-1)}}, \tag{5.84}$$

and the sequence u_n, $n = 0, 1, \ldots$ converges (to the solution u). The first iterate u_1 satisfies the equation

$$L(u_1) = [0, 0, \epsilon_a(t)], \tag{5.85}$$

and according to (5.18), (4.198), there exists a constant b such that

$$\|\epsilon_a\| \leq \frac{b}{a^{(m-1)}}. \tag{5.86}$$

Combining (5.85) with (5.55) and (5.86), we observe that there exist constant c_4 such that

$$\|u_1\| \leq \frac{c_4}{a^{(m-1)}}. \tag{5.87}$$

Now, we choose a constant $A > 0$ such that

$$a \cdot c_1(c_2 \cdot a + c_3)\|u_1\| \leq \frac{1}{4} \tag{5.88}$$

for all $a \geq A$. Defining $u_{-1} = 2u_1$ for convenience, we prove by induction that

$$\begin{aligned} \|u_{n+1} - u_n\| &\leq \frac{1}{2}\|u_n - u_{n-1}\|, && (5.89)\\ \|u_{n+1}\| &\leq 2\|u_1\|, && (5.90) \end{aligned}$$

for all $n \geq 0$, $a \geq A$.

The case $n = 0$ is a trivial one. For $n \geq 1$, (5.83) indicates that

$$L(u_{n+1} - u_n) = N(u_n) - N(u_{n-1}), \tag{5.91}$$

Due to Lemma 5.3, there exist continuous functions $\delta_1, \delta_2 : [0,1] \times [-a, a] \to C$, $\delta_3 : [0,1] \to C$ such that

$$N(u_n) - N(u_{n-1}) = [\delta_1(x,k), \delta_2(x,k), \int_0^x \delta_3(t)dt], \tag{5.92}$$

Now, combining (5.91), (5.92) with (5.55), (5.44), and the assumption of the induction, we obtain

$$
\begin{aligned}
\|u_{n+1} - u_n\| &\leq c_2 \cdot a \max\left(\|\delta_1\|, \|\delta_2\|\right) + c_3\|\delta_3\| \\
&\leq a \cdot c_1(c_2 \cdot a + c_3) \max\left(\|u_n\|, \|u_{n-1}\|\right) \|u_n - u_{n-1}\| \\
&\leq \frac{1}{2}\|u_n - u_{n-1}\|, \qquad (5.93)
\end{aligned}
$$

which proves (5.89). The estimate (5.90) is a direct consequence of (5.89).

Finally, the sequence u_n, $n = 0, 1, \ldots$ converges to the solution u due to (5.89), and therefore

$$\|u\| \leq \frac{2c_4}{a^{(m-1)}}, \qquad (5.94)$$

for all $a \geq A$ due to (5.90), (5.87), which was to be proved. □

Remark 5.5 *The proof above requires that $q \in c^m(R)$, with $m \geq 4$. At the expense of a considerable increase in the complexity of the proof, it is not difficult to extend this result to $m \geq 2$. However, our numerical experiments (see the following chapter) indicate that the scheme works quite well for continuous, piecewise continuously differentiable q, and even for piecewise continuously differentiable q with finite number of jumps. In the latter two cases, the rates of convergence of the algorithm are $1/a$ and $1/\sqrt{a}$, respectively.*

Chapter 6

Implementation and Numerical Results

6.1 Implementation

In implementing the algorithm of this thesis (see Chapter 5.2), the integral

$$\int_{-a}^{a}(p_+(x,k) - p_-(x,k))dk \tag{6.1}$$

in equation (5.9) is approximated by the trapezoidal sum

$$\begin{aligned} T(h) &= h\sum_{j=-M+1}^{M-1}(p_+(x,k_j) - p_-(x,k_j)) \\ &\quad + \frac{h}{2}((p_+(x,-a) - p_-(x,-a)) + (p_+(x,a) - p_-(x,a))), \end{aligned} \tag{6.2}$$

with $h = a/M,\ k_j = jh,\ j = -M, \ldots, M$. Since for real k, $p_+(x,-k) = \overline{p_+(x,k)}$, $p_-(x,-k) = \overline{p_-(x,k)}$ (see Observation (4.8)), the ODEs (5.7), (5.8), (5.9) are discretized in the k-space using $M+1$ nodes $k_j = jh,\ j = 0, \ldots, M$, leading to a system of $2M+3$ ODEs

$$p'_{h+}(x,k_j) = -ik_j\left(p^2_{h+}(x,k_j) - (1 + q_h(x))\right), \tag{6.3}$$

$$p'_{h-}(x,k_j) = ik_j\left(p^2_{h-}(x,k_j) - (1 + q_h(x))\right), \tag{6.4}$$

$$\begin{aligned} q'_h(x) &= \frac{4h}{\pi}(1 + q_h(x))\left(\sum_{j=1}^{M-1} Re(p_{h+}(x,k_j) - p_{h-}(x,k_j))\right. \\ &\quad \left. + \frac{1}{2}Re\{p_{h+}(x,0) - p_{h-}(x,0) + p_{h+}(x,a) - p_{h-}(x,a)\}\right) \end{aligned} \tag{6.5}$$

subject to the initial conditions

$$
\begin{aligned}
p_{h+}(0,k_j) &= p_0(k_j), & (6.6)\\
p_{h-}(0,k_j) &= 1, & (6.7)\\
q_h(0) &= 0 & (6.8)
\end{aligned}
$$

(see (5.10)- (5.12)). These ODEs are then solved using a standard 4-th order Runge-Kutta scheme.

When an integral is discretized via a quadrature formula, the rate of convergence of the quadrature is critical to the numerical performance of the algorithm. It turns out that while the estimate

$$\overline{p_+(x,k)} - p_-(x,k) = O(a^{-m}) \tag{6.9}$$

(see Theorem 4.18) ensures a rapid convergence of q_a to q as a grows (see Theorem 5.1), it also guarantees a rapid convergence of the trapezoidal quadrature (6.2) to the integral (6.1). This fact is formalized in the following lemma. Its proof is based on the Euler-Maclaurin summation formula (see, for example, [10]), and is omitted, since it is quite involved, and incidental to the purpose of this thesis.

Lemma 6.1 *Suppose that $q \in c_0^m([0,1])$, $m \geq 2$, $q^{(m)}$ is absolutely continuous and $q(x) > -1$ for all $x \in R$. Then there exist positive numbers c_n, $n = 0, \ldots$ such that*

$$\left| \frac{d^n \left(\overline{p_+(x,a)} - p_-(x,a)\right)}{dk^n} \right| \leq \frac{c_n}{|k|^m}. \tag{6.10}$$

Furthermore, for any $\beta > 0, b > 0$, there exists a constant $c > 0$ such that

$$\left| \int_{-a}^{a} (p_+(x,k) - p_-(x,k))dk - T\left(\frac{b}{a^\beta}\right) \right| \leq \frac{c}{a^m}. \tag{6.11}$$

Using the estimate (6.11), and reproducing the proof of Theorem 5.1 almost verbatim, one can prove the following theorem.

Theorem 6.2 *Suppose that $q \in c_0^m([0,1])$, $m \geq 4$, $q^{(m)}$ is absolutely continuous and $q(x) > -1$ for all $x \in R$. Suppose further that for given $r > 0, s > 0$, $q(r,s,x)$ denotes the soluiion q_h of the system (6.3)- (6.8) with $h = r/a^s$. Then for any $\alpha > 0, \beta > 0$, there exist constants $A > 0, c > 0$ such that*

$$|q(x) - q(\alpha,\beta,x)| \leq \frac{c}{a^{(m-1)}}. \tag{6.12}$$

for all $x \in [0,1]$, $a \geq A$

6.2 Numerical Results

We have applied the algorithm of this thesis to the reconstruction of several types of scatterers, from infinitely differentiable q to discontinuous q. The computations were performed in double precision on a SPARC 1 computer without the use of the accelerator. The results of numerical experiments for four classes of scatterers are presented in this chapter.

In the first class (Examples 1–2.2) are scatterers satisfying the smoothness conditions of Theorem 6.2. In the second class (Example 3) is a scatterer q violating the smoothness conditions only mildly (it is continuous, but its derivative is discontinuous at two points). In the third class (Examples 4.1, 4.2) are scatterers that strongly violate the smoothness conditions by being discontinuous. Finally, in Example 6 a scatterer with an index of diffraction that changes in several order of magnitude is reconstructed. As is well-known, scatterers of this type are difficult to recover due to strong back scattering.

We also performed a crude test, in Example 5, of stability of the algorithm by truncating the scattering data $p_0(k_j)$, $j = 1, \ldots, M$ after $1, 2$, or 3 digits. The truncated scattering data are subsequently used in reconstructions.

In Tables 6.1– 6.9, h_k denotes step size of the trapezoidal rule in the k-interval $[0, a]$, N_x denotes the number of points in the x-interval $[0, 2\pi]$, E^2, E^∞ represent the relative L^2 and maximum norm of error of the reconstructed scatterer, respectively. In Figures 6.1– 6.15, dotted lines denote the exact solution, while solid lines denote the numerical reconstruction. In all examples, for a given a, h_k and N_x were chosen such that further decrease of h_k and increase of N_x brought no improvements on the accuracy of the reconstruction.

Remark 6.3 *In order to obtain the scattering data $p_+(0, k)$ for the Examples 1–3, the scattered field ϕ_{scat+} was obtained as a solution of the boundary value problem (2.10), (2.8), (2.9) via a high order algorithm described in [15]. The parameters in the scheme were chosen in such a manner that at least 14-digit accuracy was always maintained. Formulae (2.4), (2.30) were then used to obtain $p_+(0, k)$ from ϕ_{scat+}.*

In Examples 4.1 and 4.2, a standard procedure for the solution of the initial value problem (2.1), (2.26) (for ϕ_+) with piecewise constant q was used (see, for example, [16]). Here, the solutions were obtained with at least 15 correct digits. The scattering data $p_+(0, k)$ were obtained from ϕ_+ via formula (2.30).

Remark 6.4 *In the examples below, no effort was made to optimize the code used, either from the algorithmic or from the programming point of view. For example, we used the Runge-Kutta scheme to solve ODEs (6.3), (6.4), (6.5). While it produced satisfactory results in our experiments, it is by no means the most efficient scheme for the solution of problems of this type.*

a	h_k	N_x	E^2	E^∞	t (sec.)
5	0.1	80	0.146×10^{-2}	0.153×10^{-2}	0.600
10	0.1	300	0.354×10^{-5}	0.415×10^{-5}	4.41
10	0.05	600	0.177×10^{-5}	0.183×10^{-5}	16.7
10	0.05	1200	0.175×10^{-5}	0.184×10^{-5}	34.2
20	0.05	2400	0.759×10^{-9}	0.108×10^{-8}	141
20	0.05	4000	0.988×10^{-10}	0.143×10^{-9}	235
20	0.025	4000	0.982×10^{-10}	0.142×10^{-9}	498

Table 6.1: CPU Times and Accuracies for Example 1

Example 1. Reconstruction of a Gaussian distribution

$$q(x) = e^{-\left(\frac{x-\pi}{\sigma}\right)^2} \tag{6.13}$$

where the variant σ given by the formula

$$\sigma = \frac{\pi}{4}\sqrt{\log_{10}(e)} = 0.5175854235\ldots \tag{6.14}$$

was chosen such that the function is effectively zero to double precision outside the interval $[0, 2\pi]$. The results of this numerical experiment are depicted in Table 6.1 and Figure 6.1. For all practical purposes, the scatterer (6.13) is a c^∞-function in R with the support on the interval $[0, 2\pi]$, and therefore the algorithm converges extremely rapidly, as demonstrated in Figure 6.1 where the two graphs of the exact q and the reconstructed q are almost identical.

In the following two examples, we reconstruct oscillatory scatterers of the form

$$q(x) = \sum_{j=1}^{3} c_j(1 - \cos(n_j x)), \tag{6.15}$$

with $n_j, c_j,\ j = 1, 2, 3$ given below. For given n_j, the coefficients c_j were chosen in such a manner that q is five times continuously differentiable for all $x \in R$, so that the rapid convergence of the reconstruction algorithm is guaranteed (see Theorems 5.1, 6.2)

Example 2.1. A less complicated scatterer is given by the formula

$$q(x) = 0.3\left((1 - \cos(2x)) - \frac{16}{21}(1 - \cos(3x)) + \frac{5}{28}(1 - \cos(4x))\right). \tag{6.16}$$

Reconstructions were performed with $a = 7,\ 14$. The results of this experiment are depicted in Table 6.2 and Figure 6.2 Since the scatterer is smooth, $\overline{p_+(x,k)}-$

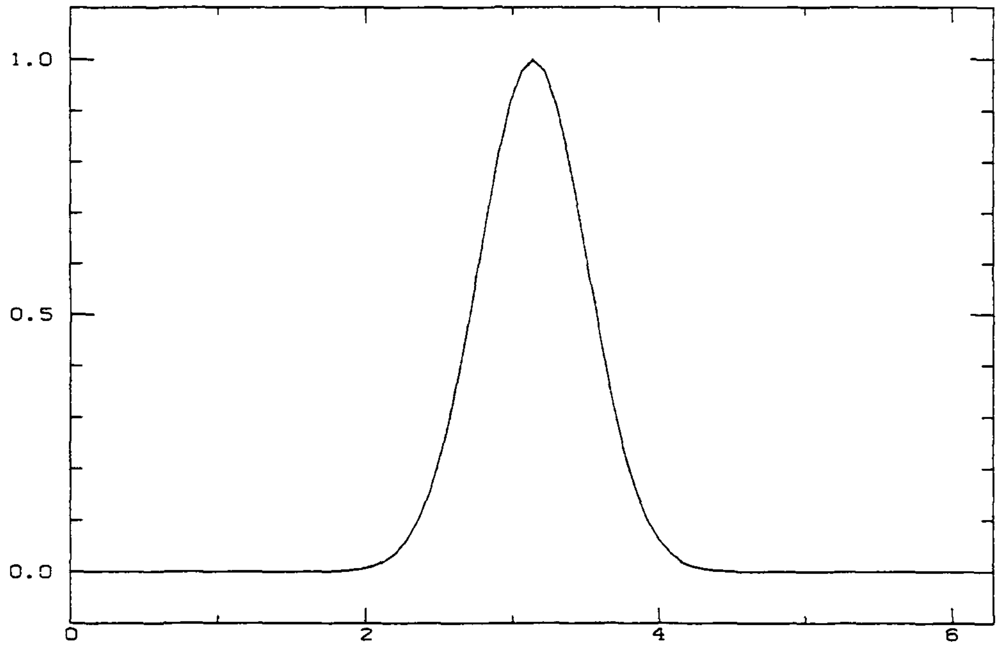

Figure 6.1: Reconstruction of Example 1 with $a = 5$

a	h_k	N_x	E^2	E^∞	t (sec.)
7	0.1	100	0.523×10^{-2}	0.983×10^{-2}	1.05
7	0.05	600	0.516×10^{-2}	0.833×10^{-2}	11.9
14	0.1	300	0.648×10^{-4}	0.172×10^{-3}	6.04
14	0.05	600	0.568×10^{-4}	0.948×10^{-4}	23.7
28	0.05	2000	0.231×10^{-7}	0.625×10^{-7}	170
28	0.025	4000	0.106×10^{-7}	0.155×10^{-7}	243

Table 6.2: CPU Times and Accuracies for Example 2.1

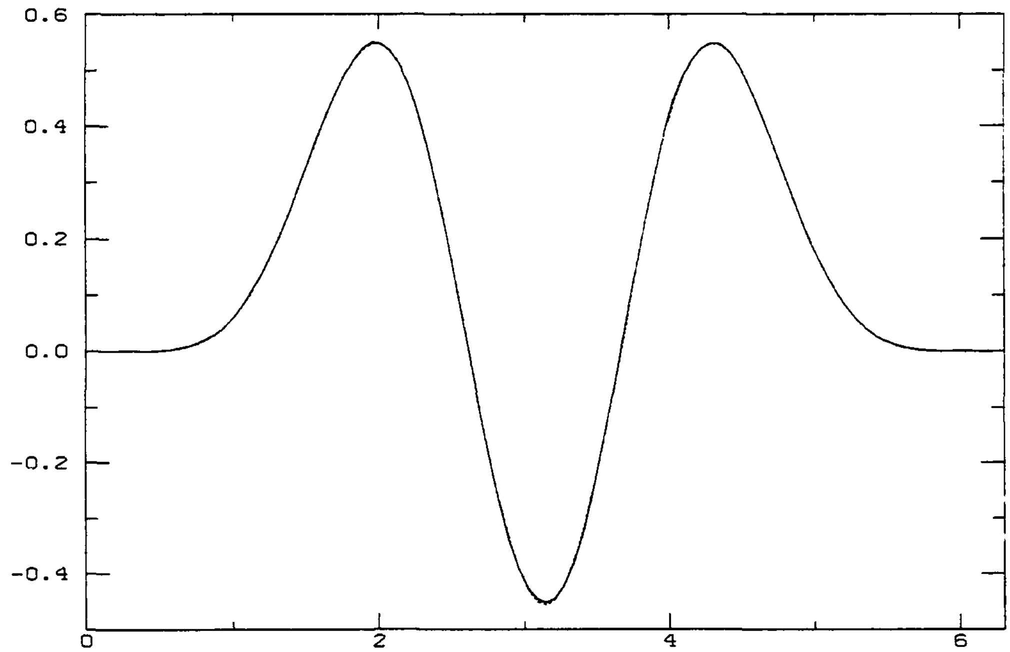

Figure 6.2: Reconstruction of Example 2.1 with $a = 7$

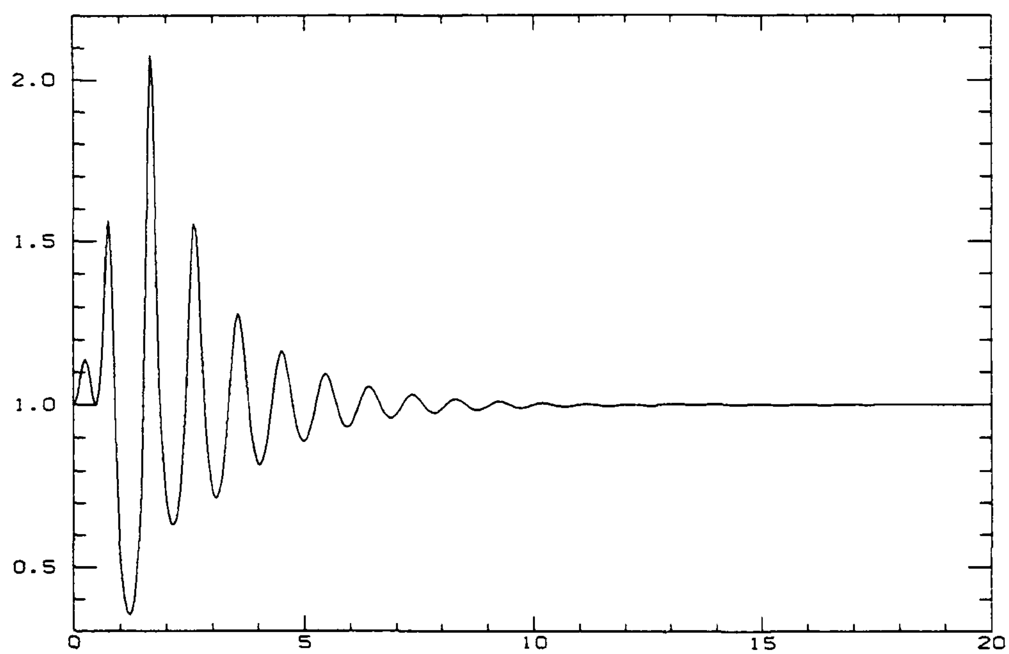

Figure 6.3: Real Part of the Scattering Data $p_0(k)$ in Example 2.1

a	h_k	N_x	E^2	E^∞	t (sec.)
10	0.1	300	0.288×10^{-1}	0.376×10^{-1}	4.41
10	0.025	600	0.281×10^{-1}	0.367×10^{-1}	35.3
10	0.025	1200	0.281×10^{-1}	0.367×10^{-1}	70.4
20	0.1	400	0.395×10^{-2}	0.754×10^{-2}	11.4
20	0.025	800	0.127×10^{-2}	0.226×10^{-2}	98.7
20	0.025	1600	0.127×10^{-2}	0.220×10^{-2}	197
40	0.025	800	0.788×10^{-4}	0.300×10^{-3}	202
40	0.025	1600	0.878×10^{-5}	0.290×10^{-4}	404

Table 6.3: CPU Times and Accuracies for Example 2.2

a	h_k	N_x	E^2	E^∞	t (sec.)
5	0.1	75	0.482×10^{-1}	0.829×10^{-1}	0.590
10	0.1	150	0.239×10^{-1}	0.462×10^{-1}	2.19
20	0.1	300	0.119×10^{-1}	0.283×10^{-1}	8.47

Table 6.4: CPU Times and Accuracies for Example 3

$p_-(x,k)$ decays rapidly as k grows. In particular, the scattering data $Re(p_0(k))$ approaches 1 rapidly, as can be seen in Figure 6.3.

Example 2.2. A more complicated scatterer is given by the formula

$$q(x) = 0.4\left((1-\cos(3x)) - \frac{1215}{2783}(1-\cos(11x)) + \frac{7}{23}(1-\cos(12x))\right). \quad (6.17)$$

Reconstructions were performed with $a = 10,\ 20$. The results of this experiment are depicted in Table 6.3 and Figure 6.4.

Example 3. In this example, we reconstruct a scatterer defined by the formula

$$q(x) = 0.2 \cdot \sin(x). \quad (6.18)$$

Note that q' is discontinuous at the points $x = 0, 2\pi$, and as a result $\overline{p_+(x,k)} - p_-(x,k)$ decays like $1/k$, as can be seen in Figure 6.6. We have not proven a convergence theorem for such scatterers, but the algorithm seems to perform quite well in this case, and its rate of convergence to be linear (see Table 6.4 and Figure 6.5).

Example 4.1. Here, we reconstruct a scatterer defined by the formula

$$q(x) = \begin{cases} 0.4 & \text{if } x \in [1,2], \\ 0 & \text{otherwise.} \end{cases} \quad (6.19)$$

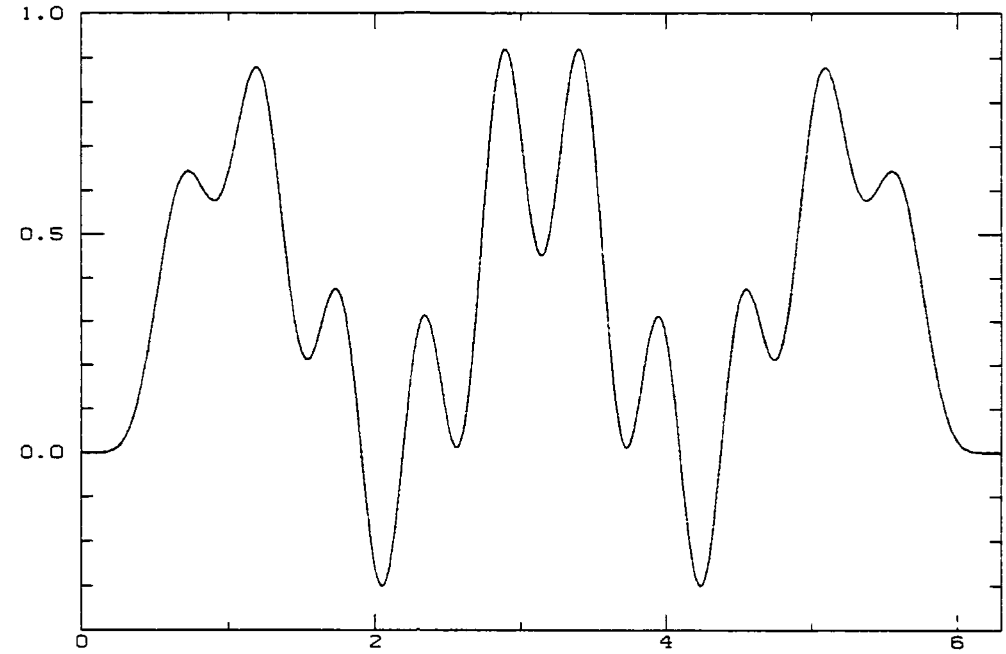

Figure 6.4: Reconstruction of Example 2.2 with $a = 20$

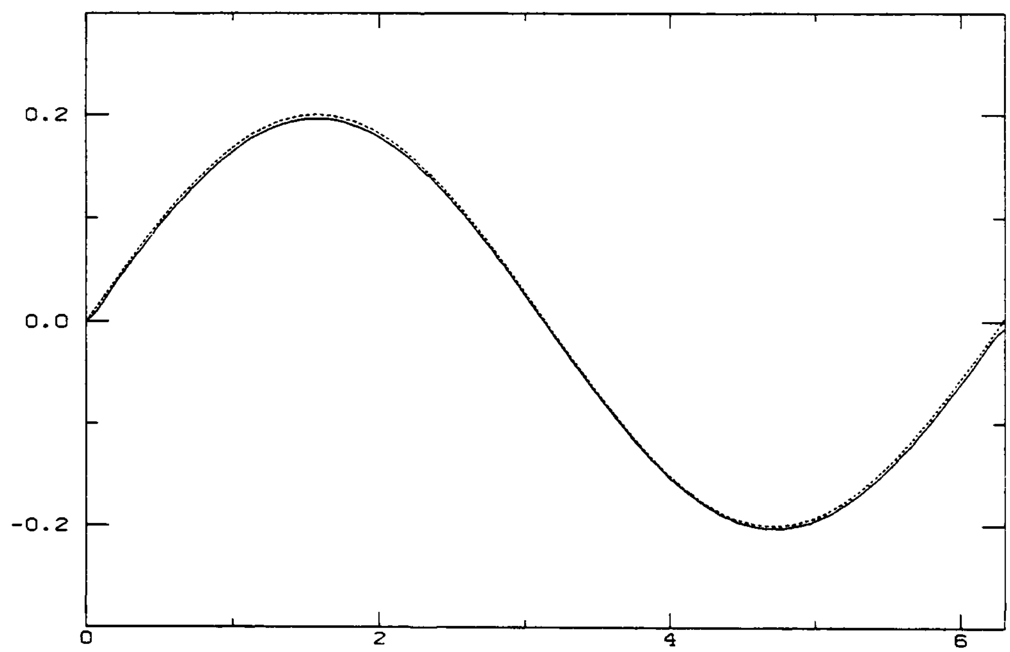

Figure 6.5: Reconstruction of Example 3 with $a = 10$

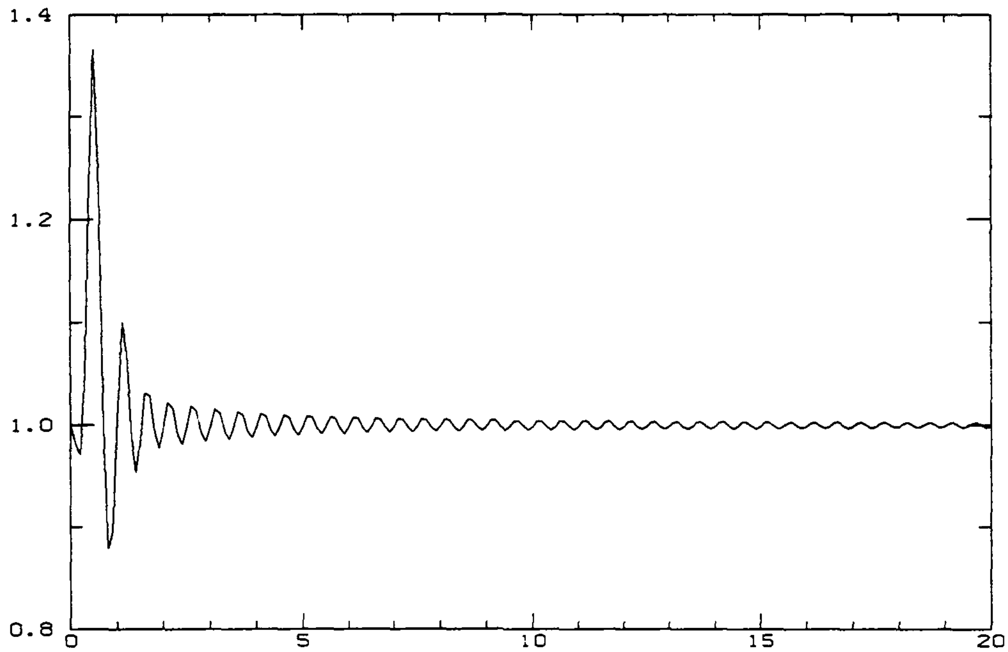

Figure 6.6: Real Part of the Scattering Data $p_0(k)$ in Example 3

a	h_k	N_x	E^2	t (sec.)
10	0.4	50	0.165	0.230
20	0.4	200	0.119	1.51
40	0.4	400	0.843×10^{-1}	6.03

Table 6.5: CPU Times and Accuracies for Example 4.1

In this example, the scatterer is discontinuous, and the conditions of Theorems 5.1, 6.2 are violated. In fact, the integrand $p_+ - p_-$ does not even converge to zero as $k \to \infty$. The results of this experiment are depicted in Figures 6.7, 6.8, and Table 6.5.

Example 4.2. In this example, we reconstruct a staircase-shaped scatterer

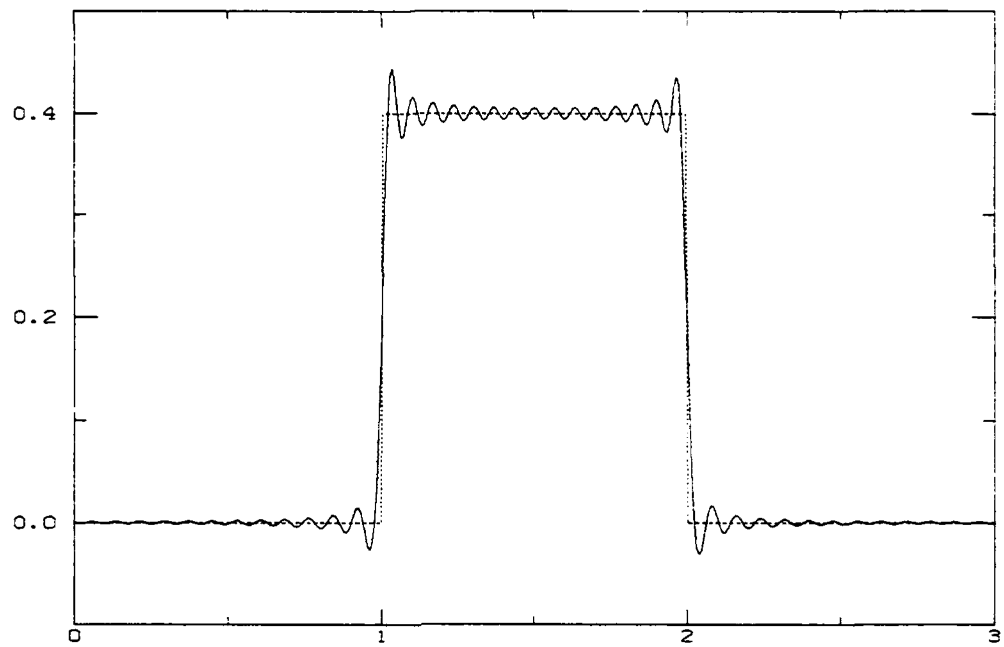

Figure 6.7: Reconstruction of Example 4.1 with $a = 40$

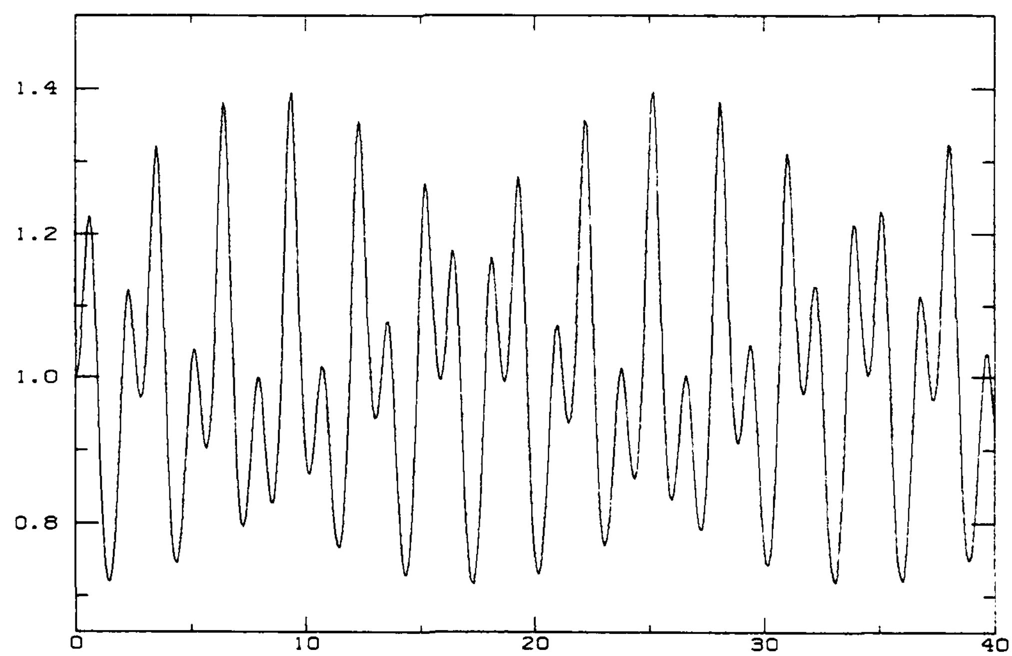

Figure 6.8: Real Part of the Scattering Data $p_0(k)$ in Example 4.1

a	h_k	N_x	E^2	t (sec.)
5	0.2	100	0.149	0.430
10	0.2	150	0.936×10^{-1}	1.18
20	0.2	300	0.682×10^{-1}	4.40

Table 6.6: CPU Times and Accuracies for Example 4.2

defined by the formula

$$q(x) = \begin{cases} 0 & x \in (-\infty, 0.5] \\ 0.1 & x \in (0.5, 1.0] \\ 0.2 & x \in (1.0, 1.5] \\ 0.4 & x \in (1.5, 2.0] \\ 0.6 & x \in (2.0, 2.5] \\ 0.5 & x \in (2.5, 3.0] \\ 0.3 & x \in (3.0, 3.5] \\ 0.1 & x \in (3.5, 4.0] \\ -0.1 & x \in (4.0, 4.5] \\ -0.3 & x \in (4.5, 5.0] \\ -0.2 & x \in (5.0, 5.5] \\ -0.1 & x \in (5.5, 6.0] \\ 0 & x \in (6.0, \infty) \end{cases} \tag{6.20}$$

This example is similar to the preceding one, but the shape of the scatterer is more complicated. The results of this experiment are shown in Table 6.6 and Figure 6.9.

Example 5. We investigate the sensitivity of the reconstruction to perturbations of the initial data. In a somewhat crude test, we perturb the initial data for the algorithm by truncating it after a specified number of decimal digits (both the real and the imaginary parts). Clearly, after such a truncation, the maximum relative error is of the order 10^{D-1} (for example, when the number 1.999 is truncated after $D = 1$ digits, the result is 1).

Tables 6.7 and 6.8 demonstrate the numerical results of the reconstruction of Examples 2.1 and 3, respectively, with various truncations of the input data. In each case, a was chosen sufficiently large that the error from the truncation of the trace formula due to finite a (see (4.194), (4.198)) is negligible compared to the error due to the finite number D of digits retained. For a given a, the parameters h_k, N_x were chosen such that accuracy of the reconstruction was not improved by a further decrease of h_k and/or increase of N_x. Also see Figures 6.10– 6.14, comparing the scatterers reconstructed using the perturbed data with the prescribed ones.

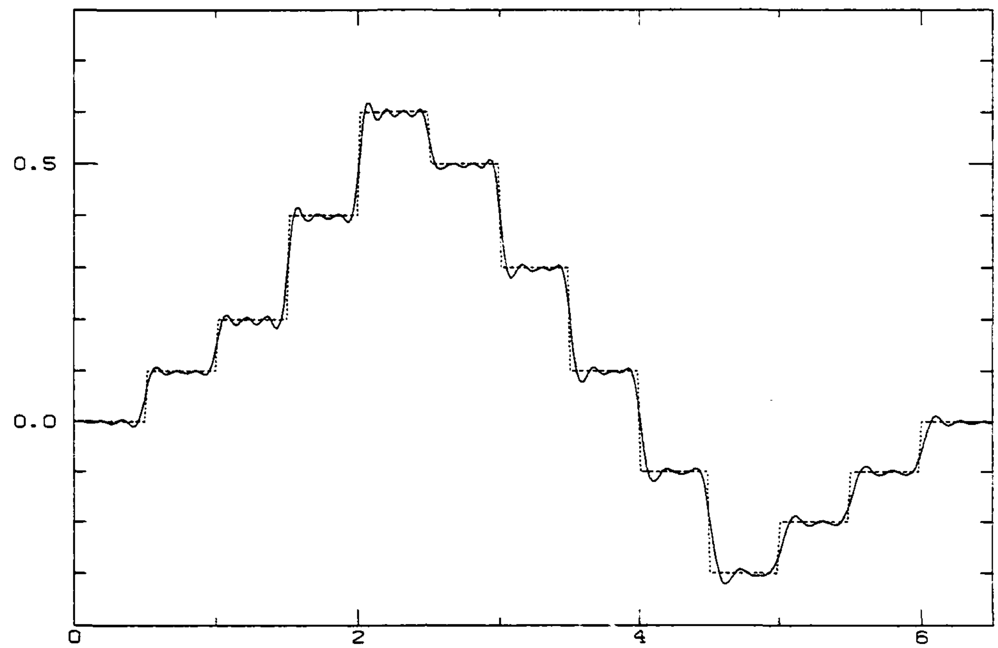

Figure 6.9: Reconstruction of Example 4.2 with $a = 20$

D	a	h_k	N_x	E^2	E^∞
1	7	0.1	100	0.410	0.474
1	14	0.1	300	0.412	0.473
2	7	0.1	100	0.126	0.156
2	14	0.1	300	0.128	0.157
3	7	0.1	100	0.174×10^{-1}	0.265×10^{-1}
3	14	0.1	300	0.187×10^{-1}	0.256×10^{-1}
4	14	0.1	300	0.126×10^{-2}	0.151×10^{-2}
4	28	0.05	600	0.118×10^{-2}	0.132×10^{-2}
5	14	0.1	300	0.297×10^{-3}	0.426×10^{-3}
5	28	0.05	600	0.250×10^{-3}	0.324×10^{-3}

Table 6.7: CPU Times and Accuracies for Example 2.1 with Truncated Data

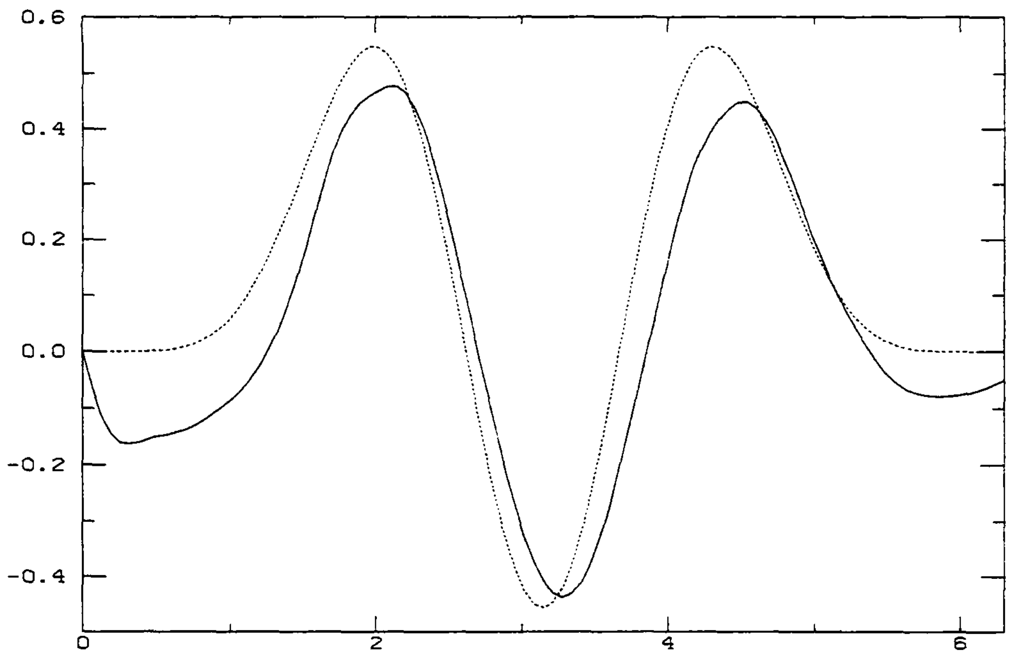

Figure 6.10: Reconstruction of Example 2.1 with $D = 1$

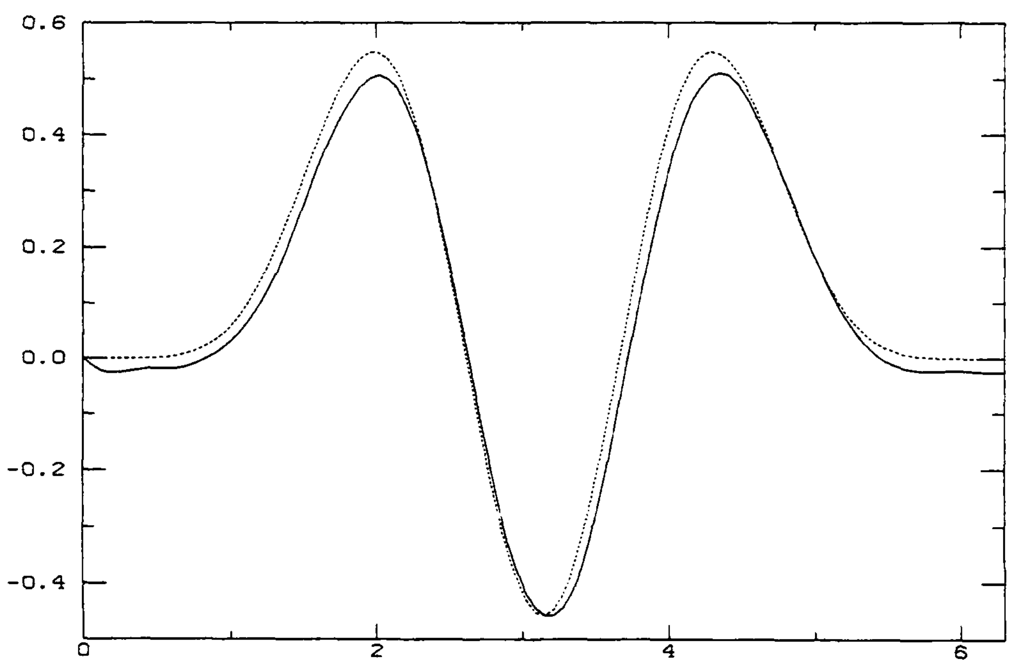

Figure 6.11: Reconstruction of Example 2.1 with $D = 2$

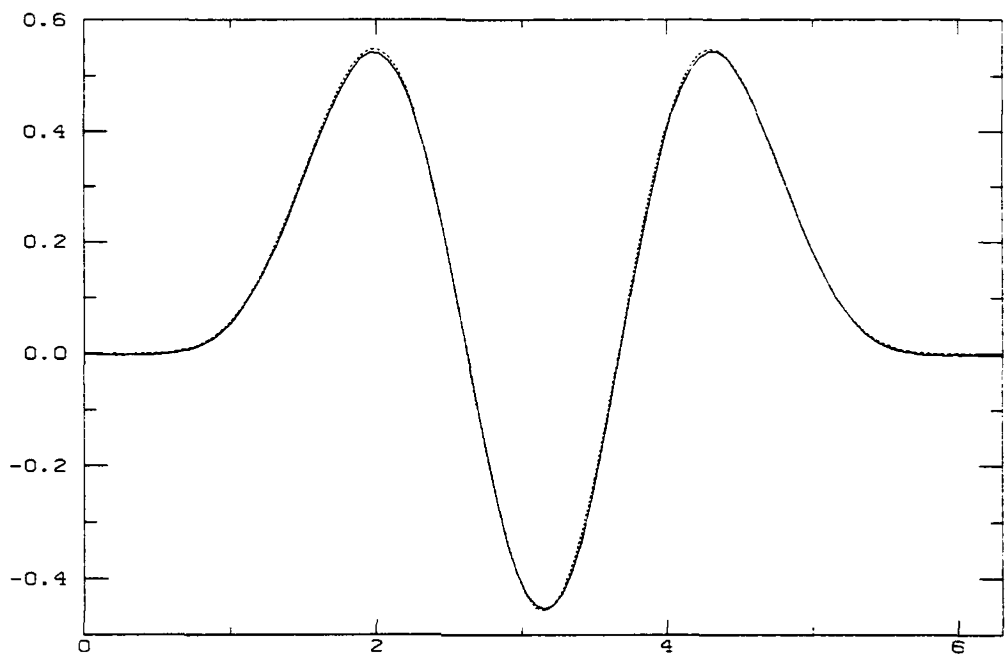

Figure 6.12: Reconstruction of Example 2.1 with $D = 3$

D	a	h_k	N_x	E^2	E^∞
1	10	0.1	150	0.647	0.863
1	20	0.1	300	0.640	0.852
2	10	0.1	150	0.121	0.173
2	20	0.1	300	0.113	0.164
3	10	0.1	150	0.314×10^{-1}	0.602×10^{-1}
3	20	0.1	300	0.206×10^{-1}	0.439×10^{-1}

Table 6.8: CPU Times and Accuracies for Example 3 with Truncated Data

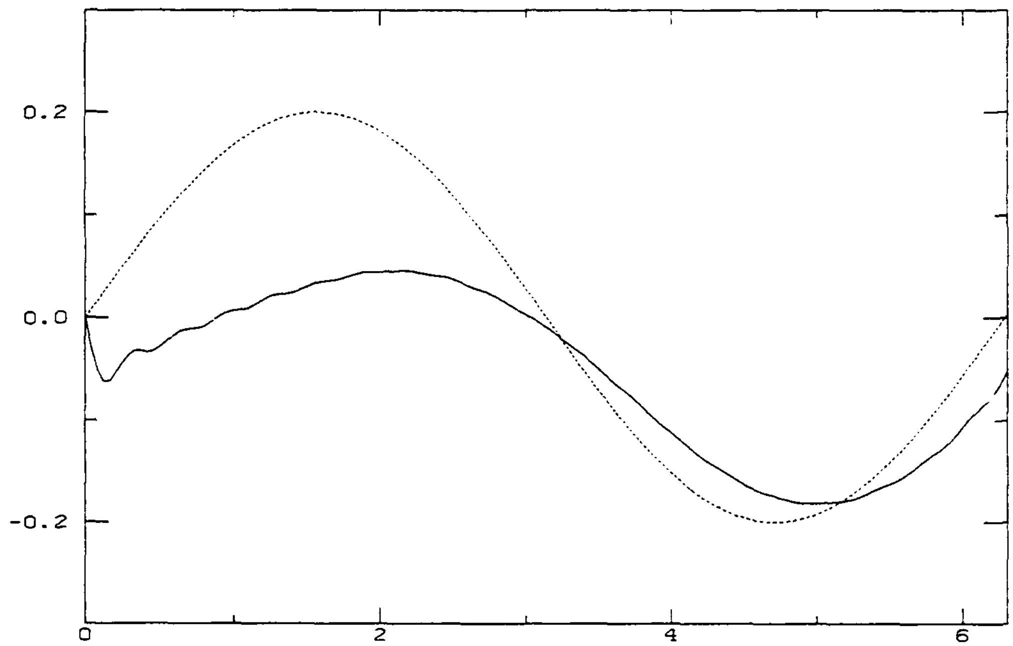

Figure 6.13: Reconstruction of Example 3 with $D = 1$

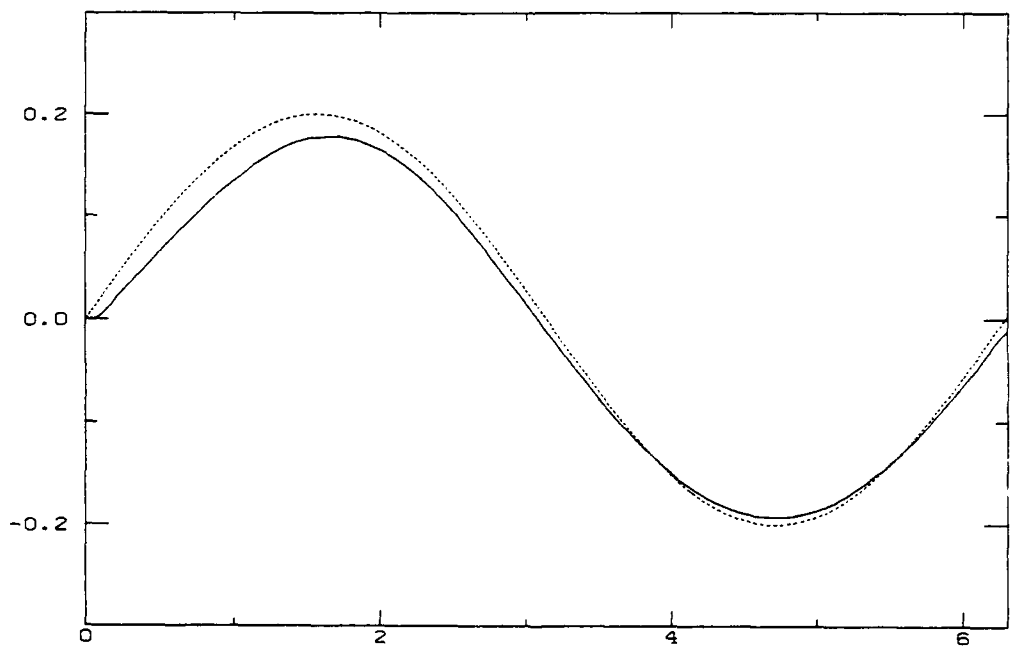

Figure 6.14: Reconstruction of Example 3 with $D = 2$

a	h_k	N_x	E^2	E^∞	t (sec.)
25	0.2	250	0.750×10^{-1}	0.153	22.6
25	0.1	250	0.722×10^{-1}	0.145	45.0
50	0.2	500	0.512×10^{-1}	0.793×10^{-1}	89.8
50	0.1	500	0.349×10^{-1}	0.686×10^{-1}	179
100	0.1	1000	0.158×10^{-1}	0.359×10^{-1}	718

Table 6.9: CPU Times and Accuracies for Example 6

We conclude the numerical examples by a nearly singular problem with the scattering potential defined by the formula

$$q(x) = 2 \cdot e^{-5\cdot(x-0.9\pi)^2} + \sin(5(2x-\pi)) \cdot \sin^2(2x-\pi). \tag{6.21}$$

The parameters in (6.21) were chosen such that the minimum of the function $1+q$ is nearly zero. In fact,

$$\min_{x\in R} q(x) = -0.9953, \tag{6.22}$$

$$\max_{x\in R} q(x) = 2.10. \tag{6.23}$$

Such a scattering potential is extremely difficult to reconstruct since the speed of sound in the scatterer changes drastically (the ratio between the maximum and minimum speed of sound is about 400), and the impedance functions p_+, p_- have large values, making the ODE system (6.3), (6.4), (6.5) stiff. A standard second order Crank-Nicolson implicit scheme was employed to solve this problem.

Example 6. Table 6.9 demonstrates the numerical results of the reconstruction of the scattering potential (6.21). Also see Figure 6.15 for the numerical reconstruction.

The following observations can be made from Tables 6.1- 6.9 and Figures 6.1- 6.15.

1. When the scatterer satisfies the conditions of Theorems 5.1, 6.2, the accuracy of the reconstruction is somewhat better than that predicated by these theorems (see Example 2.1). This indicates that (as expected) the estimates (5.13), (6.12) are somewhat pessimistic.

2. When the scatterer violates the conditions of Theorems 5.1, 6.2 mildly (by having discontinuous derivative at the points 0, 2π), the reconstruction algorithm still converges. Qualitatively, the reconstructions in Figure 3(a) should be described as good. A careful examination of Table 6.4 (and other data not presented in this thesis) shows that the error of the reconstruction for such scatterers is proportional to $1/a$.

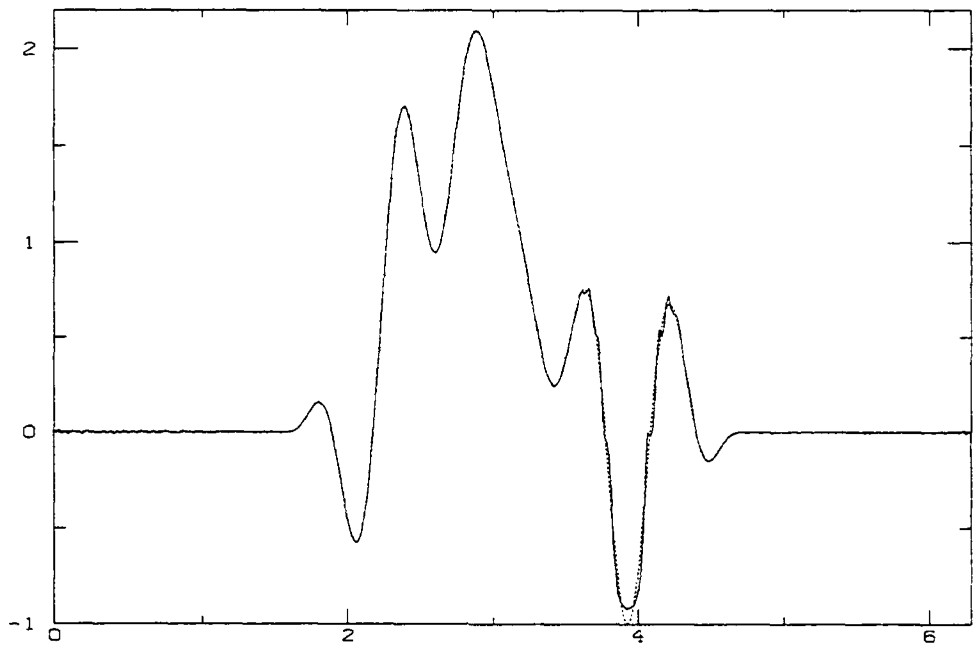

Figure 6.15: Reconstruction of Example 6 with $a = 50$

3. When the scatterer is discontinuous (Examples 4.1, 4.2), the algorithm produces results depicted in Figures 6.7, 6.9. The oscillatory behavior near the discontinuities resembles the well known Gibbs phenomenon. A careful examination of Tables 6.5, 6.6, (and other data not presented in this thesis) shows that in this case, the point-wise convergence is absent. In the L^2-norm, the error of the reconstruction behaves like $1/\sqrt{a}$.

4. When the initial data are perturbed, the resulting error of the reconstruction appears to be proportional to the magnitude of the perturbation, and the proportionality coefficient is close to 1. This is a much better estimate than the one of Lemma 5.4 which bounds the condition number of the algorithm by a. Qualitatively, it can be said that the algorithm is not sensitive to errors in the initial data.

5. When the speed of sound to be reconstructed varies by several order of magnitude, the algorithm encounters a mild difficulty in the form of stiffness of the system of equations (6.3)- (6.5). The problem is easily solved by switching to an implicit ODE solver.

Chapter 7

Generalizations and Conclusions

7.1 Generalizations in One Dimension

Following is a discussion of possible generalizations of the techniques and results of this thesis in one dimension.

1. In their present form, Theorems 5.1, 6.2 require that the scatterer have at least four continuous derivatives. Numerical examples 3–4 of the preceding section make it abundantly clear that this is a superfluous requirement. Obviously, Theorems 5.1, 6.2 can be generalized to at least include the scatterers of the type reconstructed in examples 3–4. Including the scatterers of examples 3–4 will be somewhat more involved, and will require a significant reformulation of Theorems 5.1, 6.2.

2. The algorithm of this thesis can be extended to the Schrödinger equation. The generalization is fairly straightforward and will be reported at a later date.

3. In this thesis, we reconstruct a scalar potential q given the scattering data for a single Helmholtz equation. In many problems of physical interest, the potential has several components (such as the compressional and shear speeds of sound in a medium), and the scattered data correspond to a system of Helmholtz equations (such as equations of elastic scattering, or Maxwell's equations in the frequency domain). An extension of the techniques to these cases appears to be relatively straightforward, and will be reported at a later date.

4. The impedance function formulation of the inverse problem (see, for example, Section 5.2) can be reformulated as an initial value problem for two variables called local reflection coefficients $R_+(x,k)$ and $R_-(x,k)$ defined below. Later in Section 7.2, an extension of this formulation to two dimensions will be presented.

For any $x_0 \in [0,1]$ ($[0,1]$ is the support of the scatterer q), we define the

truncated scatterers $q_r(x)$ and $q_l(x)$ by the formulas

$$q_r(x) = \begin{cases} 0 & \text{if } x < x_0, \\ q(x) & \text{if } x \geq x_0, \end{cases} \tag{7.1}$$

$$q_l(x) = \begin{cases} q(x) & \text{if } x < x_0, \\ 0 & \text{if } x \geq x_0. \end{cases} \tag{7.2}$$

Clearly, the right-traveling incoming wave $\phi_{inc+}(x,k) = e^{ikx}$ gets reflected at $x = x_0$ due to the discontinuity of q_r at that point. Since the $q_r(x) = 0$ for all $x < x_0$, the total field, which is the solution of the Helmholtz equation, may be expressed as (see formula (2.17) in Section 2.2)

$$\phi_+(x,k) = e^{ikx} + R_+(x_0,k)e^{-ikx}, \text{ for all } x < x_0, \tag{7.3}$$

where $R_+(x_0,k)e^{-ikx}$ is the reflected (or back-scattered) wave. We refer to $R_+(x_0,k)$ as the local reflection coefficient at x_0.

Denote by p_+ and p_{+r} the impedance functions for the two scatterers q and q_r respectively (see Section 2.2 for the definition of the impedance functions). For all $x \geq x_0$, p_+ and p_{+r} satisfy the same Riccati equation (3.50), since $q_r(x) = q(x)$. Furthermore, they satisfy same initial condition (3.52); consequently

$$p_+(x,k) = p_{+r}(x,k), \text{ for all } x \geq x_0. \tag{7.4}$$

Combining formulas (2.15), (7.3), and (7.4) with the fact that $p_{+r}(x,k)$ is continuous across $x = x_0$, we have the formula

$$p_+(x_0,k) = \frac{1 - R_+(x_0,k)e^{-2ikx_0}}{1 + R_+(x_0,k)e^{-2ikx_0}}, \tag{7.5}$$

from which we obtain

$$R_+(x_0,k)e^{-2ikx_0} = \frac{1 - p_+(x_0,k)}{1 + p_+(x_0,k)}, \tag{7.6}$$

for all real x_0.

We observe that there exists a real $c > 0$ such that for all real x and complex k in the upper half of the complex k-plane,

$$|R_+(x,k)e^{-2ikx}| \leq c < 1, \tag{7.7}$$

since p_+ is uniformly bounded, and $Re(p_+) > 0$ is uniformly bounded from below by a positive number (see Theorem 4.17 in Section 4.2).

It is now clear, from the Riccati equation (3.50) and formulas (7.5), (7.5), that there is an ODE for the local reflection coefficient $R_+(x,k)$

$$R'_+(x,k) = -\frac{ik}{2}q(x)\left(R_+(x,k)e^{-ikx} + e^{ikx}\right)^2, \tag{7.8}$$

which is, of course, a Riccati equation for $R_+(x,k)$ with the variable k as a parameter.

In a similar manner, the local reflection coefficient $R_-(x,k)$ is defined by the formula

$$\phi_-(x,k) = e^{-ikx} + R_-(x_0,k)e^{ikx}, \text{ for all } x \geq x_0 1, \tag{7.9}$$

where ϕ_- is the solution of the Helmholtz equation induced by the left-traveling incoming wave $\phi_{inc-}(x,k) = e^{-ikx}$ and the scatterer q_l defined by formula (7.2). The following is a list of similar facts about R_-.

For any real x and complex k in the upper half plane, R_- is connected with p_- via the formulas

$$p_-(x,k) = \frac{1 - R_-(x,k)e^{2ikx}}{1 + R_-(x,k)e^{2ikx}}, \tag{7.10}$$

$$R_-(x,k)e^{2ikx} = \frac{1 - p_-(x,k)}{1 + p_-(x,k)}; \tag{7.11}$$

R_- is bounded by the formula

$$|R_-(x,k)e^{2ikx}| \leq c < 1; \tag{7.12}$$

and R_- satisfies the Riccati equation

$$R'_-(x,k) = \frac{ik}{2}q(x)(R_-(x,k)e^{ikx} + e^{-ikx})^2. \tag{7.13}$$

Finally, it is easy to see that there is a trace formula associated with the local reflection coefficients R_+, R_-,

$$\begin{aligned} q'(x) &= -\frac{1}{\pi}(1+q(x))\left(1+\sqrt{1+q(x)}\right) \times \\ &\int_{-\infty}^{\infty} \left(R_+(x,k)e^{-2ikx} - R_-(x,k)e^{2ikx}\right) dk. \end{aligned} \tag{7.14}$$

The ODE system (7.8), (7.13), and (7.14) for R_+, R_-, and q is solved with appropriate initial values of R_+, R_-, and q at $x = 0$. As is expected, the convergence results are similar to those presented in Section 5.2.

Numerical experiments show that the performance of the algorithm using the local reflection coefficients is slightly and consistently better than that using the impedance functions.

7.2 Extensions to Two Dimensions

The following is a brief discussion of the generalizations of our inversion algorithms in two dimensions. While the impedance function formulation of the

inverse problem (see Section 2.2) can be easily generalized in two dimensions, the reflection coefficient formulation (see Section 7.1 for the 1-D formulation) in two dimensions is not straightforward. Below, we first formulate the forward (as opposed to inverse) scattering problem in two dimensions. We then derive the Riccati equation for the impedance mappings, for the two dimensional inverse problem. A trace formula associated with the impedance mappings (similar to the trace formula used in Section 5.2) is then presented. Finally, for the generalization of the reflection coefficient formulation, we will present a Riccati equation for the scattering matrix in two dimensions.

7.2.1 Forward Scattering Problem in Two Dimensions

We first formulate the forward scattering problem in two dimensions. Let us consider the two dimensional Helmholtz equation

$$\Delta\phi(x,y) + k^2 \cdot (1 + q(x,y)) \cdot \phi(x,y) = 0. \tag{7.15}$$

where Δ is the Laplace operator. We assume that the scatterer $q : R^2 \to R$ is a smooth function and has a compact support Ω, and that $q > -1$.

In the forward scattering problem, we are interested in solutions of Helmholtz equation (7.15) of the form

$$\phi(x,y) = \phi_0(x,y) + \psi(x,y), \tag{7.16}$$

where ϕ is referred to as the total field, ϕ_0 is referred to as the incoming field, and ψ is referred to as the scattered field. We also say that the total field ϕ is induced by the incoming field ϕ_0.

The incoming field is a solution of the Helmholtz equation (7.15) with $q \equiv 0$. It can be expressed by a linear combination of the incoming plane waves of the form

$$\phi_{ipw}(x,y) = e^{ik(x\cdot\cos(\beta)+y\cdot\sin(\beta))} \tag{7.17}$$

with β the direction in which a plane wave travels. As can be easily verified, for each real β, function (7.15) is a solution of the Helmholtz equation (7.15) with $q \equiv 0$.

The scattered field ψ satisfies the so-called Sommerfeld radiation condition, or the outgoing radiation condition

$$\sqrt{r} \cdot \left(\frac{\partial\psi}{\partial r} - i \cdot k \cdot \psi \right) \to 0, \text{ as } r = \sqrt{x^2 + y^2} \to \infty \ , \tag{7.18}$$

and satisfies an inhomogeneous Helmholtz equation

$$\Delta\psi(x,y) + k^2 \cdot (1 + q(x,y)) \cdot \psi(x,y) = -k^2 \cdot q(x,y) \cdot \phi_0(x,y). \tag{7.19}$$

7.2.2 Riccati Equations for the Impedance Mappings

We define the set of right-going plane waves by the formula (see (7.17) for the definition of the incoming plane waves)

$$\Phi_{rpw} = \{e^{ik(x\cdot\cos(\beta)+y\cdot\sin(\beta))} \mid -\frac{\pi}{2} \leq \beta \leq \frac{\pi}{2}\}. \tag{7.20}$$

A solution of the Helmholtz equation (7.15) is said to be a right-going solution, if it is induced by a right-going plane wave, or in general, by a function ϕ_{+0} in the linear span of the set Φ_{rpw} of right-going plane waves (see (7.16)). Therefore, the set of right-going solutions is defined by the formula

$$\Phi_{rgs} = \{\phi_+ = \phi_{+0} + \psi_+ \mid \phi_{+0} \in \mathrm{Span}(\Phi_{rpw}), \psi \text{ is the scattered field }\}. \tag{7.21}$$

We are now ready to define the impedance mapping P_+. For fixed x and k, $P_+(x,k)$ is a linear mapping, : $L^2_{loc} \rightarrow L^2_{loc}$, where L^2_{loc} is the local L^2 space on the real line. It maps, for fixed x and k, a right-going solution $\phi_+ \in \Phi_{rgs}$ as a function of y to its derivative with respect to x as a function of y, more specificly,

$$P_+(x,k)\cdot\phi_+(x,y) = \frac{1}{ik}\cdot\frac{\partial\phi_+(x,y)}{\partial x}, \text{for any } \phi_+ \in \Phi_{rgs}. \tag{7.22}$$

Assuming that for fixed x and k, the right-going solutions in Φ_{rgs} is dense in L^2_{loc}, and combining (7.22) with the Helmholtz equation (7.15), we can easily obtain a Riccati equation for the impedance mapping P_+,

$$P'_+(x,k) = -ik\left(P^2_+(x,k) - \frac{1}{k^2}\frac{d^2}{dy^2} - (I + q(x,\cdot))\right), \tag{7.23}$$

where I is the identity operator, $q(x,\cdot)$ is a diagonal linear operator,

$$q(x,\cdot)\cdot f(y) = q(x,y)\cdot f(y), \tag{7.24}$$

for a fixed x and any $f \in L^2_{loc}$.

The impedance mapping P_- can be defined by first introducing the set of all left-going solutions in a similar manner, which leads to a Riccati equation for P_-,

$$P'_-(x,k) = ik\left(P^2_-(x,k) - \frac{1}{k^2}\frac{d^2}{dy^2} - (I + q(x,\cdot))\right). \tag{7.25}$$

These Riccati equations are operator equations; the operator $\frac{d^2}{dy^2}$, for example, in the standard discretized form, is a tridiagonal matrix, hence the term "matrix Riccati equations".

Combining the definition of the impedance mappings with the standard WKB approximation, we obtain a trace formula (the derivation is omitted here),

$$\frac{\partial q(x,y)}{\partial x} = \frac{2}{\pi}(1+q(x,y))\int_{-\infty}^{\infty}(P_+(x,k)-P_-(x,k))\cdot F_{one}(y)dk, \tag{7.26}$$

where $F_{one}(y) \equiv 1$ for any real y is clearly a function in L^2_{loc}. Numerical experiments show that when the integral is truncated so that it is taken over the interval $[-a,a]$, the rate of convergence behaves exactly like that in one dimension (see Section 4.3).

Remark 7.1 *While the matrix Riccati equation and the trace formula associated with the impedance mappings are extremely similar to their one dimensional counterparts (see Section 5.2), the spatial discretization of these two dimensional objects is quite different from that in 1-D. The fact that the scattered field ψ decays very slowly like $1/\sqrt{r}$ makes spatial truncation virtually impossible.*

In solving the initial value problem of the ODEs (7.23), (7.25), and (7.26), the desired truncation in y-direction (see Remark 7.1) is achieved by periodizing the scatterer q in y-direction (the details of this procedure are omitted). The periodized problem is then truncated in frequency space, and discretized in a procedure similar to that described in Section 6.1. Numerical experiments are presently being conducted, and the results, together with the periodizing procedure, will be reported at a later date.

7.2.3 Riccati Equations for the Scattering Matrix

In a manner similar to that in which the impedance functions p_+ and p_- are connected to the local reflection coefficients R_+ and R_- in one dimension (see Section 7.1), the two dimensional objects P_+ and P_- are related to linear mappings called the scattering matrices, which are the two dimensional analogues of the local reflection coefficients R_+ and R_-.

We will define these scattering matrices in the polar coordinates, and will present matrix Riccati equations for the scattering matrices. The procedures used here being similar to those described in Section 7.1, only the main results will be presented. We will also casually use several well established results about cylindrical functions.

For any $R > 0$, we define the truncated scatterer q_R by the formula

$$q_R(r,\theta) = \begin{cases} q(r,\theta) & \text{if } r < R, \\ 0 & \text{if } r \geq R, \end{cases} \tag{7.27}$$

We first discuss the forward scattering from the truncated scatterer q_R. As is well-known, for any r, an incoming field (see Section 7.2.1) can be expressed as the so-called Bessel-Fourier series

$$\phi_{inc}(r,\theta) = \sum_{m=-\infty}^{\infty} \alpha_m \cdot J_m(kr)e^{im\theta}. \tag{7.28}$$

Is is also well-know that for a fixed R, and for any $r > R$ where $q_R(r,\theta) = 0$, the scattered field induced by ϕ_{inc} and q_R can be written as the so-called Hankel-Fourier series

$$\psi(r,\theta) = \sum_{m=-\infty}^{\infty} \beta_m(R,k) \cdot H_m(kr)e^{im\theta}, \tag{7.29}$$

where J_m is the first kind Bessel function of order m, H_m is the first kind Hankel function of order m. It is well-known that once $m > \frac{e}{2}kr$, $J_m(kr)$ decays and $H_m(kr)$ grows like

$$\begin{aligned} J_m(kr) &\sim \frac{1}{\sqrt{2\pi m}}\left(\frac{e\cdot k\cdot r}{2m}\right)^m, & (7.30)\\ H_m(kr) &\sim -i\cdot\sqrt{\frac{2}{\pi m}}\left(\frac{e\cdot k\cdot r}{2m}\right)^{-m}. & (7.31)\end{aligned}$$

As is well-known, for an incoming field of the form (7.28), there exists a unique scattered field of the form (7.29), such that $\phi = \phi_{inc} + \psi$ is a solution of the Helmholtz equation (7.15). Consequently, the linear mapping

$$S(R,k)\cdot\{\alpha_m(R,k), m = 0,\pm1,...\} = \{\beta_m(R,k), m = 0,\pm1,...\} \tag{7.32}$$

is well-defined, and is normally referred to as the scattering matrix. Furthermore, the entries of the matrix S decay very rapidly, since $\beta_m(R,k)$ decays extremely rapidly due to (7.30), (7.31).

The scattering matrix S satisfies the Riccati equation

$$S'(r,k) = \frac{i\pi r}{2}k^2\cdot(J(kr)+S(r,k)\cdot H(kr))\cdot F\cdot q(r,\cdot)\cdot F^{-1}\cdot(J(kr)+H(kr)\cdot S(r,k)), \tag{7.33}$$

where $J(kr)$, $H(kr)$ are diagonal matrices

$$\begin{aligned} J(kr) &= diag\{J_0(kr), J_{\pm1}(kr),\ldots\}, & (7.34)\\ H(kr) &= diag\{H_0(kr), H_{\pm1}(kr),\ldots\}, & (7.35)\end{aligned}$$

$q(r,\cdot)$ is a diagonal linear operator

$$q(r,\cdot)\cdot f(\theta) = q(r,\theta)\cdot f(\theta), \tag{7.36}$$

and F is the Fourier transform.

The derivation of this Riccati equation follows the procedures outlined in Section 7.1, where Riccati equations for the local reflection coefficients are obtained from the Riccati equations for the impedance functions. The derivation is omitted here, and will be reported at a later date.

Remark 7.2 *While the investigation of the inverse scattering problem in the form of Riccati equation (7.33) is in progress, numerical experiments show that ODE (7.33) could be useful for the solution of the forward scattering problem. Unlike the Riccati equations for the impedance mappings, where there is a serious problem with truncation, the scattering matrix S can be truncated easily since its high-frequency entries (those with large indices) decay very rapidly. We currently use the standard 4-th order Runge-Kutta method to solve the forward scattering problem, that is, starting from $r = 0$ and $S(r,k) = 0$, solve the initial value problem till $r = R_0$, for some R_0 where the entire circle contains the support of the scatterer. The whole procedure, as is easy to see, requirs order $N^4 \cdot \log(N)$ operations to obtain an $N \times N$ scattering matrix.*

7.3 Conclusions

An algorithm has been presented for the solution of the inverse scattering problem for the Helmholtz equation in one dimension. The algorithm is based on a combination of the standard Riccati equation for the impedance function with a newly constructed trace formula for the derivative of the potential, and leads to extremely accurate and efficient numerical schemes for smooth scatterers. The principal differences between this scheme and various layer-stripping techniques (see [12], [13], [14]) are:

1. The algorithm operates in the frequency domain, while other efficient schemes are time-domain ones.

2. While the layer-stripping algorithms assume (at least conceptually) that the scatterer is piece-wise constant, and are best in this regime, our algorithm assumes that the scatterer is continuously differentiable. When the scatterer has a sufficient number of derivatives, the algorithm converges almost instantaneously (see Theorems 5.1, 6.2).

3. The principal drawback of the layer-stripping algorithms is the fact that they are an essentially one-dimensional techniques, and the author is not aware of any successful attempts to generalize them to higher dimensions. Our techniques do generalize to two and three dimensions, and in fact an implementation of a two-dimensional version of the procedure is in progress.

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